

CHEMISTRY

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Supporting Information

The Bonding Situation in Metalated Ylides

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1. Coordinates and Energies

1.1 BP86-D3(BJ)/Def2TZVP, equilibrium structures

All Energies are given in Hartree.

1

E = -1871.86371102

| Atomic symbol | x | y | z |
|---------------|-----------|-----------|-----------|
| C | 0.271893 | 0.330973 | -1.509916 |
| P | -0.749844 | -0.103195 | -0.231516 |
| C | -2.248604 | 0.931970 | -0.083213 |
| C | -2.534231 | 1.821538 | -1.126967 |
| C | -3.106555 | 0.855921 | 1.024565 |
| C | -3.675276 | 2.624188 | -1.065938 |
| H | -1.845814 | 1.883001 | -1.972678 |
| C | -4.245479 | 1.660534 | 1.082274 |
| H | -2.873635 | 0.186998 | 1.855003 |
| C | -4.532350 | 2.543173 | 0.035226 |
| H | -3.889985 | 3.321165 | -1.877902 |
| H | -4.907259 | 1.604234 | 1.948736 |
| H | -5.421585 | 3.174637 | 0.083605 |
| C | -0.047897 | -0.154451 | 1.451527 |
| C | 0.650201 | -1.294749 | 1.881689 |
| C | -0.014659 | 1.013310 | 2.234498 |
| C | 1.353690 | -1.276321 | 3.087943 |
| H | 0.639736 | -2.197162 | 1.267563 |
| C | 0.695102 | 1.027767 | 3.436373 |
| H | -0.520314 | 1.912392 | 1.883661 |
| C | 1.377721 | -0.115508 | 3.868398 |
| H | 1.880582 | -2.172687 | 3.422090 |
| H | 0.717061 | 1.938323 | 4.038066 |
| H | 1.923269 | -0.101988 | 4.814023 |
| C | -1.331689 | -1.802463 | -0.539267 |
| C | -2.125116 | -2.488921 | 0.392569 |
| C | -0.983386 | -2.418954 | -1.747768 |
| C | -2.564492 | -3.784327 | 0.116384 |
| H | -2.392485 | -2.017305 | 1.339623 |
| C | -1.426331 | -3.715738 | -2.021164 |
| H | -0.364352 | -1.852163 | -2.448270 |
| C | -2.216157 | -4.398981 | -1.091771 |
| H | -3.180671 | -4.315951 | 0.843942 |
| H | -1.155071 | -4.193619 | -2.964618 |
| H | -2.562974 | -5.411594 | -1.307228 |
| S | 1.196192 | 1.706350 | -1.371511 |
| O | 0.901761 | 2.648324 | -0.272418 |
| O | 1.512185 | 2.295342 | -2.675863 |
| C | 2.606258 | 0.757558 | -0.865854 |
| C | 3.373933 | 0.040379 | -1.825537 |
| C | 2.974318 | 0.655819 | 0.502242 |
| C | 4.384842 | -0.780725 | -1.413633 |
| H | 3.143963 | 0.154802 | -2.883992 |
| C | 3.986886 | -0.185446 | 0.873944 |
| H | 2.445605 | 1.244864 | 1.249244 |
| H | 5.011544 | -1.357401 | -2.091818 |
| H | 4.308050 | -0.315439 | 1.905930 |
| H | 5.430420 | -1.510968 | 0.218634 |
| N | 4.667889 | -0.908062 | -0.071440 |

1'

E = -1871.87660585

| Atomic symbol | x | y | z |
|---------------|-----------|-----------|-----------|
| C | -0.065228 | -0.209977 | -1.697312 |
| P | 0.802990 | 0.078072 | -0.281942 |
| C | 2.088239 | -1.155387 | 0.134436 |
| C | 2.351163 | -2.164062 | -0.800532 |
| C | 2.812406 | -1.111882 | 1.335802 |
| C | 3.334776 | -3.120328 | -0.537787 |
| H | 1.769432 | -2.191380 | -1.724177 |
| C | 3.793357 | -2.069545 | 1.596183 |
| H | 2.600614 | -0.340823 | 2.078637 |
| C | 4.056986 | -3.073684 | 0.657689 |
| H | 3.531727 | -3.907978 | -1.267188 |
| H | 4.351660 | -2.035234 | 2.533738 |
| H | 4.823523 | -3.823361 | 0.863256 |
| C | -0.170260 | 0.269484 | 1.252967 |
| C | -0.838419 | 1.481504 | 1.499244 |
| C | -0.419102 | -0.834775 | 2.086447 |
| C | -1.715888 | 1.596527 | 2.577279 |
| H | -0.662013 | 2.336146 | 0.843350 |
| C | -1.298645 | -0.714824 | 3.166148 |
| H | 0.071998 | -1.785876 | 1.879340 |
| C | -1.944162 | 0.500602 | 3.418210 |
| H | -2.221417 | 2.545637 | 2.765598 |
| H | -1.474228 | -1.573811 | 3.817218 |
| H | -2.620770 | 0.595625 | 4.269869 |
| C | 1.679023 | 1.663402 | -0.471891 |
| C | 2.300162 | 2.302468 | 0.611787 |
| C | 1.746422 | 2.232651 | -1.750115 |
| C | 2.985133 | 3.502679 | 0.416038 |
| H | 2.234922 | 1.874261 | 1.613498 |
| C | 2.437664 | 3.431306 | -1.942867 |
| H | 1.237497 | 1.715873 | -2.567873 |
| C | 3.057262 | 4.066717 | -0.862488 |
| H | 3.462747 | 4.000121 | 1.262240 |
| H | 2.490081 | 3.872233 | -2.940202 |
| H | 3.594871 | 5.004770 | -1.014181 |
| S | -1.176562 | -1.413634 | -1.670471 |
| O | -1.097189 | -2.456970 | -0.601572 |
| O | -1.550866 | -1.887870 | -3.003536 |
| C | -2.603308 | -0.476244 | -1.084312 |
| C | -3.167243 | 0.648475 | -1.701415 |
| C | -4.169765 | 1.345855 | -1.048449 |
| H | -2.781734 | 0.944903 | -2.675882 |
| C | -4.013421 | -0.157000 | 0.824372 |
| H | -2.582867 | -1.683627 | 0.502164 |
| H | -4.630251 | 2.213980 | -1.522588 |
| H | -4.257511 | -0.526945 | 1.817515 |
| H | -5.354830 | 1.503415 | 0.786036 |
| C | -4.590804 | 0.948315 | 0.244843 |
| N | -3.070993 | -0.849400 | 0.133068 |

1''

E = -1871.8755977

| Atomic symbol | x | y | z |
|---------------|----------|-----------|-----------|
| C | 0.013321 | -0.206941 | -1.708616 |
| P | 0.860617 | 0.036126 | -0.290518 |
| C | 1.995232 | -1.323009 | 0.157932 |

| | | | |
|---|-----------|-----------|-----------|
| C | 1.704814 | -2.611379 | -0.313207 |
| C | 3.112503 | -1.113507 | 0.980769 |
| C | 2.522897 | -3.684141 | 0.050849 |
| H | 0.838656 | -2.766222 | -0.960418 |
| C | 3.930471 | -2.187966 | 1.333991 |
| H | 3.351887 | -0.110323 | 1.336626 |
| C | 3.634495 | -3.474900 | 0.871976 |
| H | 2.291678 | -4.686323 | -0.314620 |
| H | 4.803608 | -2.020027 | 1.967237 |
| H | 4.276263 | -4.313782 | 1.148010 |
| C | -0.134058 | 0.321589 | 1.208590 |
| C | -0.897709 | 1.498498 | 1.294600 |
| C | -0.257804 | -0.660784 | 2.200917 |
| C | -1.768029 | 1.689670 | 2.365697 |
| H | -0.813703 | 2.255439 | 0.512813 |
| C | -1.129638 | -0.462379 | 3.275104 |
| H | 0.325811 | -1.579835 | 2.130132 |
| C | -1.883741 | 0.710243 | 3.358822 |
| H | -2.373574 | 2.595266 | 2.418874 |
| H | -1.221177 | -1.229445 | 4.046278 |
| H | -2.571508 | 0.860760 | 4.192605 |
| C | 1.894816 | 1.519252 | -0.465537 |
| C | 2.348023 | 2.238979 | 0.650395 |
| C | 2.257792 | 1.926618 | -1.756475 |
| C | 3.170220 | 3.354176 | 0.473182 |
| H | 2.038667 | 1.942125 | 1.654409 |
| C | 3.083088 | 3.039241 | -1.928019 |
| H | 1.867046 | 1.368721 | -2.610582 |
| C | 3.541680 | 3.751771 | -0.814845 |
| H | 3.514764 | 3.918081 | 1.341895 |
| H | 3.363786 | 3.356259 | -2.934041 |
| H | 4.182197 | 4.625067 | -0.951686 |
| S | -1.303745 | -1.061582 | -1.805990 |
| O | -1.436339 | -2.513522 | -1.566812 |
| C | -2.670207 | -0.303981 | -0.908756 |
| C | -4.087443 | 1.562977 | -0.430756 |
| H | -2.688758 | 1.511288 | -2.092338 |
| C | -4.159326 | -0.253139 | 0.961952 |
| H | -2.880176 | -1.948573 | 0.478723 |
| H | -4.470468 | 2.560560 | -0.667395 |
| H | -4.584423 | -0.715976 | 1.857777 |
| C | -3.204992 | -0.944393 | 0.208440 |
| C | -3.107703 | 0.982803 | -1.235542 |
| N | -4.611224 | 0.972946 | 0.659536 |
| O | -1.817472 | -0.818332 | -3.354530 |
| H | -2.443069 | -1.551213 | -3.535481 |

2

E = -1855.30469091

| Atomic symbol | x | y | z |
|---------------|-----------|-----------|-----------|
| C | 0.036179 | 0.115021 | -1.770062 |
| P | -0.792225 | -0.021126 | -0.350781 |
| C | -1.895553 | 1.357607 | 0.219963 |
| C | -1.499102 | 2.662376 | -0.117451 |
| C | -3.093631 | 1.163271 | 0.925786 |
| C | -2.282229 | 3.752897 | 0.272092 |
| H | -0.574019 | 2.801150 | -0.691492 |
| C | -3.881950 | 2.256314 | 1.298530 |
| H | -3.420088 | 0.153016 | 1.178208 |

| | | | |
|---|-----------|-----------|-----------|
| C | -3.474182 | 3.555338 | 0.978304 |
| H | -1.960735 | 4.764909 | 0.013539 |
| H | -4.817422 | 2.092851 | 1.840119 |
| H | -4.088933 | 4.410182 | 1.271461 |
| C | 0.130880 | -0.425070 | 1.188487 |
| C | 0.914813 | -1.593086 | 1.183705 |
| C | 0.214016 | 0.446105 | 2.283703 |
| C | 1.746928 | -1.889525 | 2.260196 |
| H | 0.882945 | -2.247807 | 0.310432 |
| C | 1.050620 | 0.147139 | 3.363792 |
| H | -0.374644 | 1.365198 | 2.284868 |
| C | 1.814880 | -1.022232 | 3.357474 |
| H | 2.366768 | -2.788009 | 2.234220 |
| H | 1.110139 | 0.835815 | 4.210356 |
| H | 2.478818 | -1.249439 | 4.194630 |
| C | -1.936259 | -1.446139 | -0.512918 |
| C | -2.429131 | -2.155991 | 0.591422 |
| C | -2.306526 | -1.837489 | -1.806448 |
| C | -3.291573 | -3.242182 | 0.404130 |
| H | -2.115587 | -1.873546 | 1.598897 |
| C | -3.177549 | -2.912318 | -1.992057 |
| H | -1.858403 | -1.289165 | -2.641235 |
| C | -3.672854 | -3.617793 | -0.886964 |
| H | -3.660377 | -3.799633 | 1.268726 |
| H | -3.464546 | -3.211152 | -3.003307 |
| H | -4.345832 | -4.466240 | -1.033853 |
| S | 1.372105 | 1.064363 | -2.001155 |
| O | 1.283909 | 2.476939 | -1.532540 |
| O | 1.882734 | 0.905660 | -3.376159 |
| C | 2.665364 | 0.343856 | -0.952575 |
| C | 3.241928 | -0.880611 | -1.315077 |
| C | 3.056594 | 0.974603 | 0.232976 |
| C | 4.210023 | -1.464800 | -0.497614 |
| H | 2.919198 | -1.354800 | -2.243439 |
| C | 4.019973 | 0.381457 | 1.054209 |
| H | 2.596163 | 1.929478 | 0.488833 |
| H | 4.662291 | -2.417571 | -0.786558 |
| H | 4.309620 | 0.869583 | 1.988067 |
| H | 5.355405 | -1.298559 | 1.336044 |
| C | 4.604306 | -0.835412 | 0.691610 |

3

E = -1379.70195405

| Atomic symbol | x | y | z |
|---------------|-----------|-----------|-----------|
| C | -1.282309 | 0.676614 | 0.000001 |
| P | 0.261315 | 0.145524 | -0.000000 |
| C | 1.185701 | 0.789842 | 1.454709 |
| C | 0.533393 | 1.705469 | 2.288340 |
| C | 2.503955 | 0.409526 | 1.747459 |
| C | 1.188313 | 2.238544 | 3.400940 |
| H | -0.495193 | 1.977030 | 2.034951 |
| C | 3.159628 | 0.942052 | 2.859747 |
| H | 3.017385 | -0.319513 | 1.118638 |
| C | 2.503609 | 1.859297 | 3.687454 |
| H | 0.671470 | 2.950825 | 4.047574 |
| H | 4.184439 | 0.638567 | 3.083215 |
| H | 3.017337 | 2.274817 | 4.556690 |
| C | 1.185699 | 0.789844 | -1.454710 |
| C | 2.503953 | 0.409530 | -1.747462 |

| | | | |
|---|-----------|-----------|-----------|
| C | 0.533388 | 1.705471 | -2.288340 |
| C | 3.159624 | 0.942058 | -2.859750 |
| H | 3.017385 | -0.319509 | -1.118641 |
| C | 1.188308 | 2.238548 | -3.400940 |
| H | -0.495197 | 1.977030 | -2.034949 |
| C | 2.503603 | 1.859303 | -3.687456 |
| H | 4.184435 | 0.638574 | -3.083219 |
| H | 0.671462 | 2.950828 | -4.047573 |
| H | 3.017330 | 2.274824 | -4.556691 |
| C | 0.716069 | -1.642904 | -0.000001 |
| C | 0.789610 | -2.353450 | 1.209699 |
| C | 0.789604 | -2.353450 | -1.209702 |
| C | 0.943761 | -3.741646 | 1.209921 |
| H | 0.728525 | -1.811864 | 2.156198 |
| C | 0.943754 | -3.741647 | -1.209924 |
| H | 0.728513 | -1.811866 | -2.156201 |
| C | 1.020565 | -4.440003 | -0.000001 |
| H | 1.006334 | -4.280677 | 2.157567 |
| H | 1.006322 | -4.280679 | -2.157570 |
| H | 1.143520 | -5.524657 | -0.000001 |
| C | -4.885148 | 0.671301 | 0.000004 |
| C | -4.653159 | -0.668803 | 0.000001 |
| H | -5.818624 | 1.221216 | 0.000005 |
| H | -5.344936 | -1.502720 | 0.000001 |
| C | -2.602678 | 0.371542 | 0.000002 |
| N | -3.274415 | -0.856610 | -0.000000 |
| N | -3.651254 | 1.309274 | 0.000004 |
| C | -3.420943 | 2.734785 | 0.000006 |
| H | -2.328838 | 2.869680 | 0.000006 |
| H | -3.849309 | 3.208214 | -0.897476 |
| H | -3.849308 | 3.208211 | 0.897491 |
| C | -2.583666 | -2.122945 | -0.000003 |
| H | -1.939110 | -2.214940 | -0.887256 |
| H | -1.939109 | -2.214944 | 0.887249 |
| H | -3.322698 | -2.933221 | -0.000005 |

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E = -1339.81565116

| Atomic symbol | x | y | z |
|---------------|-----------|-----------|-----------|
| C | 1.020595 | 1.362694 | -0.235510 |
| P | -0.211379 | 0.269696 | -0.054884 |
| C | -0.289403 | -0.745126 | 1.512339 |
| C | 0.369808 | -0.211971 | 2.627805 |
| C | -0.927630 | -1.987516 | 1.627445 |
| C | 0.375951 | -0.897642 | 3.843505 |
| H | 0.890275 | 0.742571 | 2.503168 |
| C | -0.924815 | -2.677686 | 2.844302 |
| H | -1.411870 | -2.426131 | 0.751400 |
| C | -0.275902 | -2.132007 | 3.956646 |
| H | 0.901218 | -0.477179 | 4.705261 |
| H | -1.425048 | -3.646959 | 2.924164 |
| H | -0.268092 | -2.672785 | 4.906587 |
| C | -0.434609 | -1.050855 | -1.322938 |
| C | -1.403460 | -0.975249 | -2.339430 |
| C | 0.552276 | -2.057950 | -1.398519 |
| C | -1.411304 | -1.897128 | -3.388687 |
| H | -2.158110 | -0.186276 | -2.302967 |
| C | 0.545580 | -2.970567 | -2.454517 |
| H | 1.345873 | -2.071243 | -0.646029 |

| | | | |
|---|-----------|-----------|-----------|
| C | -0.438345 | -2.903766 | -3.449729 |
| H | -2.181416 | -1.832328 | -4.162462 |
| H | 1.320035 | -3.740883 | -2.504946 |
| H | -0.441975 | -3.624049 | -4.271695 |
| C | -1.803347 | 1.162050 | -0.037706 |
| C | -3.016026 | 0.524560 | 0.272101 |
| C | -1.801290 | 2.531824 | -0.333525 |
| C | -4.214475 | 1.248852 | 0.268575 |
| H | -3.022616 | -0.539319 | 0.516909 |
| C | -2.996068 | 3.253728 | -0.335881 |
| H | -0.823860 | 2.978472 | -0.546888 |
| C | -4.209364 | 2.612146 | -0.037690 |
| H | -5.154481 | 0.745935 | 0.510552 |
| H | -2.987367 | 4.321707 | -0.569805 |
| H | -5.145403 | 3.176791 | -0.039097 |
| C | 4.256762 | -0.188881 | 0.018780 |
| C | 4.623520 | 1.117259 | -0.233799 |
| H | 4.917368 | -1.041012 | 0.176942 |
| H | 5.589387 | 1.604836 | -0.331663 |
| C | 2.359966 | 0.915166 | -0.182633 |
| N | 3.430446 | 1.813046 | -0.367342 |
| N | 2.891528 | -0.326872 | 0.051915 |
| C | 3.268006 | 3.218559 | -0.634222 |
| H | 2.180582 | 3.384993 | -0.704568 |
| H | 3.681640 | 3.841707 | 0.179370 |
| H | 3.752163 | 3.509529 | -1.583251 |

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E = -1935.65844227

| Atomic symbol | x | y | z |
|---------------|-----------|-----------|-----------|
| C | -0.249573 | 1.136750 | -0.312061 |
| P | 1.212138 | 0.381647 | -0.090721 |
| C | 1.363523 | -0.682243 | 1.392302 |
| C | 0.846645 | -1.990492 | 1.379587 |
| C | 1.747879 | -0.111014 | 2.617945 |
| C | 0.709120 | -2.705792 | 2.570272 |
| H | 0.526582 | -2.440826 | 0.439016 |
| C | 1.607655 | -0.829184 | 3.807530 |
| H | 2.146762 | 0.905197 | 2.635205 |
| C | 1.083495 | -2.126846 | 3.787529 |
| H | 0.296446 | -3.715828 | 2.545340 |
| H | 1.907781 | -0.374710 | 4.753865 |
| H | 0.969277 | -2.685548 | 4.718208 |
| C | 2.568432 | 1.596454 | 0.077932 |
| C | 3.914337 | 1.209772 | 0.154365 |
| C | 2.226338 | 2.951372 | 0.152230 |
| C | 4.909886 | 2.174979 | 0.313782 |
| H | 4.185921 | 0.154406 | 0.087836 |
| C | 3.224955 | 3.917173 | 0.305721 |
| H | 1.166054 | 3.211711 | 0.083903 |
| C | 4.565727 | 3.529912 | 0.389431 |
| H | 5.957066 | 1.872365 | 0.375260 |
| H | 2.956617 | 4.974211 | 0.360367 |
| H | 5.346340 | 4.283622 | 0.510725 |
| C | 1.760276 | -0.681620 | -1.482196 |
| C | 2.646514 | -1.758210 | -1.334415 |
| C | 1.250454 | -0.377467 | -2.752752 |
| C | 3.008576 | -2.527677 | -2.443768 |
| H | 3.039338 | -2.011033 | -0.347864 |

| | | | |
|---|-----------|-----------|-----------|
| C | 1.620427 | -1.139802 | -3.861335 |
| H | 0.547868 | 0.455575 | -2.842882 |
| C | 2.497249 | -2.219695 | -3.707712 |
| H | 3.688164 | -3.373176 | -2.319449 |
| H | 1.220165 | -0.896096 | -4.847533 |
| H | 2.779441 | -2.822978 | -4.572730 |
| P | -1.615997 | 0.553108 | 0.419956 |
| C | -3.059366 | 1.526678 | -0.100411 |
| C | -2.889511 | 2.508212 | -1.085130 |
| C | -4.332949 | 1.289079 | 0.438737 |
| C | -3.986135 | 3.252917 | -1.525228 |
| H | -1.882583 | 2.664580 | -1.481264 |
| C | -5.427199 | 2.034975 | -0.003713 |
| H | -4.459963 | 0.524073 | 1.206605 |
| C | -5.255089 | 3.016623 | -0.986084 |
| H | -3.851795 | 4.019147 | -2.291466 |
| H | -6.417617 | 1.850365 | 0.417075 |
| H | -6.112663 | 3.597351 | -1.331926 |
| C | -2.033429 | -1.199561 | 0.070696 |
| C | -1.660903 | -1.706659 | -1.184761 |
| C | -2.593531 | -2.067119 | 1.020501 |
| C | -1.821889 | -3.060156 | -1.478935 |
| H | -1.208550 | -1.031607 | -1.912318 |
| C | -2.743765 | -3.426308 | 0.729221 |
| H | -2.888177 | -1.675301 | 1.994501 |
| C | -2.353989 | -3.926663 | -0.516296 |
| H | -1.517177 | -3.442766 | -2.454860 |
| H | -3.162533 | -4.098467 | 1.481236 |
| H | -2.465840 | -4.989704 | -0.738660 |
| N | -1.820811 | 0.551910 | 2.132819 |
| H | -1.747846 | 1.509983 | 2.485617 |
| H | -1.080470 | 0.000441 | 2.580033 |

6

E = -1935.08887155

| Atomic symbol | x | y | z |
|---------------|-----------|-----------|-----------|
| C | 0.305094 | 1.103290 | -0.601611 |
| P | -1.130715 | 0.446068 | -0.164298 |
| C | -2.139654 | -0.524439 | -1.391734 |
| C | -1.448197 | -1.098291 | -2.470268 |
| C | -3.528906 | -0.705373 | -1.294511 |
| C | -2.138207 | -1.858455 | -3.420217 |
| H | -0.363165 | -0.935734 | -2.568853 |
| C | -4.217458 | -1.453519 | -2.253477 |
| H | -4.081186 | -0.256013 | -0.467488 |
| C | -3.521381 | -2.038281 | -3.317409 |
| H | -1.585842 | -2.307742 | -4.249592 |
| H | -5.299906 | -1.582400 | -2.169546 |
| H | -4.058653 | -2.626693 | -4.065756 |
| C | -2.277911 | 1.780967 | 0.369511 |
| C | -3.368173 | 1.575197 | 1.227757 |
| C | -2.019417 | 3.071291 | -0.112437 |
| C | -4.193363 | 2.644910 | 1.592893 |
| H | -3.554497 | 0.579550 | 1.636163 |
| C | -2.848713 | 4.136863 | 0.241503 |
| H | -1.134096 | 3.196762 | -0.744606 |
| C | -3.939773 | 3.926339 | 1.095570 |
| H | -5.032778 | 2.477341 | 2.272488 |
| H | -2.640697 | 5.139385 | -0.140971 |

| | | | |
|---|-----------|-----------|-----------|
| H | -4.584352 | 4.761743 | 1.380157 |
| C | -1.148946 | -0.697750 | 1.282196 |
| C | -1.221754 | -2.089437 | 1.121151 |
| C | -0.878493 | -0.176207 | 2.558996 |
| C | -1.039747 | -2.939963 | 2.214561 |
| H | -1.404692 | -2.506974 | 0.129879 |
| C | -0.723196 | -1.024162 | 3.655509 |
| H | -0.779013 | 0.905293 | 2.679999 |
| C | -0.803832 | -2.412249 | 3.486306 |
| H | -1.067720 | -4.021804 | 2.067462 |
| H | -0.524788 | -0.603891 | 4.644824 |
| H | -0.659920 | -3.078982 | 4.339630 |
| P | 1.652151 | 0.236470 | -1.175209 |
| C | 3.102019 | 1.286310 | -0.694475 |
| C | 2.952815 | 2.416636 | 0.119490 |
| C | 4.379691 | 0.950532 | -1.168049 |
| C | 4.061709 | 3.200664 | 0.457249 |
| H | 1.940984 | 2.653613 | 0.463551 |
| C | 5.490960 | 1.723767 | -0.823301 |
| H | 4.475692 | 0.082562 | -1.825919 |
| C | 5.334591 | 2.852949 | -0.008424 |
| H | 3.935041 | 4.084509 | 1.089145 |
| H | 6.483670 | 1.451677 | -1.192890 |
| H | 6.202925 | 3.461580 | 0.257976 |
| C | 1.969323 | -1.262806 | -0.158457 |
| C | 2.183533 | -1.157421 | 1.224999 |
| C | 1.893365 | -2.536744 | -0.739337 |
| C | 2.327225 | -2.300628 | 2.010652 |
| H | 2.221794 | -0.166207 | 1.682140 |
| C | 2.028871 | -3.683955 | 0.049334 |
| H | 1.735633 | -2.590279 | -1.818855 |
| C | 2.250481 | -3.570363 | 1.425405 |
| H | 2.478462 | -2.204292 | 3.088283 |
| H | 1.964637 | -4.673071 | -0.413077 |
| H | 2.350800 | -4.465950 | 2.043759 |
| N | 1.810731 | -0.323352 | -2.679497 |
| H | 1.549675 | 0.413368 | -3.345062 |

7

E = -1484.13439637

| Atomic symbol | x | y | z |
|---------------|-----------|-----------|-----------|
| C | 0.305094 | 1.103290 | -0.601611 |
| P | -1.130715 | 0.446068 | -0.164298 |
| C | -2.139654 | -0.524439 | -1.391734 |
| C | -1.448197 | -1.098291 | -2.470268 |
| C | -3.528906 | -0.705373 | -1.294511 |
| C | -2.138207 | -1.858455 | -3.420217 |
| H | -0.363165 | -0.935734 | -2.568853 |
| C | -4.217458 | -1.453519 | -2.253477 |
| H | -4.081186 | -0.256013 | -0.467488 |
| C | -3.521381 | -2.038281 | -3.317409 |
| H | -1.585842 | -2.307742 | -4.249592 |
| H | -5.299906 | -1.582400 | -2.169546 |
| H | -4.058653 | -2.626693 | -4.065756 |
| C | -2.277911 | 1.780967 | 0.369511 |
| C | -3.368173 | 1.575197 | 1.227757 |
| C | -2.019417 | 3.071291 | -0.112437 |
| C | -4.193363 | 2.644910 | 1.592893 |
| H | -3.554497 | 0.579550 | 1.636163 |

| | | | |
|---|-----------|-----------|-----------|
| C | -2.848713 | 4.136863 | 0.241503 |
| H | -1.134096 | 3.196762 | -0.744606 |
| C | -3.939773 | 3.926339 | 1.095570 |
| H | -5.032778 | 2.477341 | 2.272488 |
| H | -2.640697 | 5.139385 | -0.140971 |
| H | -4.584352 | 4.761743 | 1.380157 |
| C | -1.148946 | -0.697750 | 1.282196 |
| C | -1.221754 | -2.089437 | 1.121151 |
| C | -0.878493 | -0.176207 | 2.558996 |
| C | -1.039747 | -2.939963 | 2.214561 |
| H | -1.404692 | -2.506974 | 0.129879 |
| C | -0.723196 | -1.024162 | 3.655509 |
| H | -0.779013 | 0.905293 | 2.679999 |
| C | -0.803832 | -2.412249 | 3.486306 |
| H | -1.067720 | -4.021804 | 2.067462 |
| H | -0.524788 | -0.603891 | 4.644824 |
| H | -0.659920 | -3.078982 | 4.339630 |
| P | 1.652151 | 0.236470 | -1.175209 |
| C | 3.102019 | 1.286310 | -0.694475 |
| C | 2.952815 | 2.416636 | 0.119490 |
| C | 4.379691 | 0.950532 | -1.168049 |
| C | 4.061709 | 3.200664 | 0.457249 |
| H | 1.940984 | 2.653613 | 0.463551 |
| C | 5.490960 | 1.723767 | -0.823301 |
| H | 4.475692 | 0.082562 | -1.825919 |
| C | 5.334591 | 2.852949 | -0.008424 |
| H | 3.935041 | 4.084509 | 1.089145 |
| H | 6.483670 | 1.451677 | -1.192890 |
| H | 6.202925 | 3.461580 | 0.257976 |
| C | 1.969323 | -1.262806 | -0.158457 |
| C | 2.183533 | -1.157421 | 1.224999 |
| C | 1.893365 | -2.536744 | -0.739337 |
| C | 2.327225 | -2.300628 | 2.010652 |
| H | 2.221794 | -0.166207 | 1.682140 |
| C | 2.028871 | -3.683955 | 0.049334 |
| H | 1.735633 | -2.590279 | -1.818855 |
| C | 2.250481 | -3.570363 | 1.425405 |
| H | 2.478462 | -2.204292 | 3.088283 |
| H | 1.964637 | -4.673071 | -0.413077 |
| H | 2.350800 | -4.465950 | 2.043759 |
| N | 1.810731 | -0.323352 | -2.679497 |
| H | 1.549675 | 0.413368 | -3.345062 |

8

E = -1167.66116971

| Atomic symbol | x | y | z |
|---------------|-----------|-----------|-----------|
| C | 0.053055 | 0.034261 | 2.368759 |
| P | -0.028062 | 0.009535 | 0.727436 |
| C | 0.604316 | -1.466787 | -0.181383 |
| C | -0.236636 | -2.513122 | -0.600284 |
| C | 1.998919 | -1.662610 | -0.236533 |
| C | 0.297938 | -3.708472 | -1.085835 |
| H | -1.319729 | -2.383982 | -0.542833 |
| C | 2.532265 | -2.858511 | -0.716841 |
| H | 2.663767 | -0.872012 | 0.119049 |
| C | 1.685449 | -3.886993 | -1.150588 |
| H | -0.371711 | -4.506912 | -1.416890 |
| H | 3.616455 | -2.993167 | -0.748757 |
| H | 2.103872 | -4.823611 | -1.526266 |

| | | | |
|---|-----------|-----------|-----------|
| C | 0.799102 | 1.379363 | -0.237207 |
| C | 1.223256 | 1.280733 | -1.571214 |
| C | 1.037934 | 2.568125 | 0.466505 |
| C | 1.862506 | 2.356895 | -2.194731 |
| H | 1.068478 | 0.347667 | -2.118404 |
| C | 1.671902 | 3.646121 | -0.154686 |
| H | 0.731135 | 2.608039 | 1.516469 |
| C | 2.084002 | 3.544445 | -1.489031 |
| H | 2.193469 | 2.268394 | -3.233208 |
| H | 1.856524 | 4.566604 | 0.405110 |
| H | 2.587178 | 4.384436 | -1.974479 |
| C | -1.775463 | 0.147164 | 0.213336 |
| C | -2.155422 | 0.286159 | -1.130172 |
| C | -2.758979 | 0.114606 | 1.210165 |
| C | -3.509349 | 0.374004 | -1.473878 |
| H | -1.391802 | 0.324856 | -1.909587 |
| C | -4.109394 | 0.206679 | 0.867458 |
| H | -2.404424 | 0.019575 | 2.242734 |
| C | -4.488663 | 0.332535 | -0.477306 |
| H | -3.799297 | 0.479821 | -2.522389 |
| H | -4.872867 | 0.180440 | 1.649275 |
| H | -5.545821 | 0.403274 | -0.745919 |
| C | 1.210928 | -0.056625 | 3.103789 |
| N | 2.162818 | -0.122037 | 3.816087 |

9

E = -2111.41451385

| Atomic symbol | x | y | z |
|---------------|-----------|-----------|-----------|
| C | -0.000000 | 0.000000 | 1.220459 |
| P | 1.452168 | -0.059236 | 0.418484 |
| P | -1.452168 | 0.059236 | 0.418484 |
| C | 1.765252 | -1.564411 | -0.585934 |
| C | 2.820514 | -0.032786 | 1.623703 |
| C | -1.765252 | 1.564409 | -0.585937 |
| C | 1.826090 | 1.347365 | -0.699085 |
| C | -2.820515 | 0.032790 | 1.623701 |
| C | -1.826090 | -1.347367 | -0.699082 |
| C | 1.126453 | -2.740302 | -0.162270 |
| C | 1.271864 | -3.921392 | -0.887611 |
| C | 2.054999 | -3.940349 | -2.046671 |
| C | 2.703281 | -2.776266 | -2.468288 |
| C | 2.516376 | 0.153034 | 2.976645 |
| C | 3.542853 | 0.189704 | 3.924194 |
| C | 2.563875 | -1.591931 | -1.738415 |
| C | 4.873326 | 0.038573 | 3.520876 |
| C | 5.178398 | -0.152218 | 2.168161 |
| C | 4.154196 | -0.189162 | 1.220461 |
| C | -1.126453 | 2.740301 | -0.162276 |
| C | -1.271864 | 3.921390 | -0.887619 |
| C | -2.054999 | 3.940345 | -2.046679 |
| C | -2.703282 | 2.776261 | -2.468293 |
| C | -2.563876 | 1.591927 | -1.738418 |
| C | 1.325821 | 1.376372 | -2.011314 |
| C | 1.403921 | 2.538285 | -2.778568 |
| C | 1.985857 | 3.691784 | -2.244689 |
| C | 2.491039 | 3.673237 | -0.940992 |
| C | 2.410228 | 2.510330 | -0.172150 |
| C | -2.516378 | -0.153029 | 2.976644 |
| C | -3.542855 | -0.189696 | 3.924192 |

| | | | |
|---|-----------|-----------|-----------|
| C | -4.873328 | -0.038563 | 3.520874 |
| C | -5.178399 | 0.152226 | 2.168159 |
| C | -4.154196 | 0.189167 | 1.220459 |
| C | -2.410227 | -2.510331 | -0.172146 |
| C | -2.491036 | -3.673240 | -0.940985 |
| C | -1.985854 | -3.691790 | -2.244681 |
| C | -1.403918 | -2.538291 | -2.778563 |
| C | -1.325820 | -1.376377 | -2.011312 |
| H | -0.868869 | -0.481108 | -2.433072 |
| H | -0.998813 | -2.546559 | -3.791960 |
| H | -2.041528 | -4.603760 | -2.841716 |
| H | -2.949196 | -4.570058 | -0.518963 |
| H | -2.794750 | -2.503609 | 0.849620 |
| H | -0.493735 | 2.699159 | 0.726530 |
| H | -0.758251 | 4.826001 | -0.558008 |
| H | -2.157974 | 4.861980 | -2.622798 |
| H | -3.317920 | 2.787864 | -3.370821 |
| H | -3.066142 | 0.684180 | -2.076983 |
| H | -1.463879 | -0.264276 | 3.251144 |
| H | -3.304814 | -0.335233 | 4.979860 |
| H | -5.675460 | -0.065552 | 4.261149 |
| H | -6.216474 | 0.275574 | 1.853462 |
| H | -4.391782 | 0.342476 | 0.165640 |
| H | 3.066142 | -0.684184 | -2.076982 |
| H | 3.317919 | -2.787870 | -3.370816 |
| H | 2.157974 | -4.861985 | -2.622789 |
| H | 0.758251 | -4.826003 | -0.557999 |
| H | 0.493735 | -2.699158 | 0.726536 |
| H | 3.304811 | 0.335242 | 4.979861 |
| H | 1.463877 | 0.264280 | 3.251144 |
| H | 4.391783 | -0.342472 | 0.165642 |
| H | 6.216473 | -0.275564 | 1.853465 |
| H | 5.675458 | 0.065564 | 4.261152 |
| H | 0.868871 | 0.481103 | -2.433074 |
| H | 2.794750 | 2.503610 | 0.849616 |
| H | 2.949199 | 4.570055 | -0.518972 |
| H | 2.041533 | 4.603753 | -2.841726 |
| H | 0.998816 | 2.546551 | -3.791966 |

1.2 BP86-D3(BJ)/Def2TZVP, linear structures

1

E = -1871.85498610

| Atomic symbol | x | y | z |
|---------------|-----------|-----------|-----------|
| C | 0.292898 | -0.133312 | 1.322714 |
| P | -0.762347 | -0.008899 | 0.098787 |
| C | -1.810533 | -1.492570 | -0.123516 |
| C | -1.571612 | -2.564647 | 0.747276 |
| C | -2.796856 | -1.601693 | -1.115179 |
| C | -2.318545 | -3.739630 | 0.626550 |
| H | -0.795762 | -2.455791 | 1.510951 |
| C | -3.535072 | -2.780117 | -1.237339 |
| H | -2.990827 | -0.771212 | -1.795571 |
| C | -3.297226 | -3.849087 | -0.365591 |
| H | -2.134582 | -4.570590 | 1.310062 |
| H | -4.300056 | -2.865036 | -2.011602 |
| H | -3.879191 | -4.767910 | -0.460521 |

| | | | |
|---|-----------|-----------|-----------|
| C | 0.166029 | 0.189989 | -1.454985 |
| C | 0.622490 | 1.462798 | -1.837383 |
| C | 0.584201 | -0.941549 | -2.173885 |
| C | 1.464149 | 1.601974 | -2.942358 |
| H | 0.305751 | 2.340368 | -1.271277 |
| C | 1.429618 | -0.798368 | -3.276045 |
| H | 0.235047 | -1.930176 | -1.870644 |
| C | 1.870867 | 0.472555 | -3.662686 |
| H | 1.798752 | 2.595776 | -3.247101 |
| H | 1.736649 | -1.680310 | -3.841931 |
| H | 2.513555 | 0.584980 | -4.538676 |
| C | -1.896214 | 1.421234 | 0.185434 |
| C | -2.625601 | 1.890697 | -0.917620 |
| C | -2.004339 | 2.070378 | 1.422764 |
| C | -3.470123 | 2.993963 | -0.777029 |
| H | -2.514845 | 1.414937 | -1.894102 |
| C | -2.857916 | 3.167032 | 1.561887 |
| H | -1.394871 | 1.714652 | 2.258162 |
| C | -3.592285 | 3.627622 | 0.464345 |
| H | -4.030397 | 3.363637 | -1.638055 |
| H | -2.942114 | 3.668956 | 2.527466 |
| H | -4.253529 | 4.489517 | 0.572390 |
| S | 1.344576 | -0.257305 | 2.542505 |
| O | 1.458964 | -1.585508 | 3.157054 |
| O | 1.423974 | 0.891419 | 3.450962 |
| C | 2.540662 | -0.089878 | 1.249462 |
| C | 2.978961 | 1.197198 | 0.822514 |
| C | 2.989555 | -1.233023 | 0.525215 |
| C | 3.689734 | 1.315330 | -0.338325 |
| H | 2.709442 | 2.074663 | 1.408495 |
| C | 3.697845 | -1.062789 | -0.630111 |
| H | 2.728691 | -2.227802 | 0.883093 |
| H | 4.025082 | 2.267660 | -0.744915 |
| H | 4.038072 | -1.886095 | -1.255436 |
| H | 4.484420 | 0.310124 | -1.960150 |
| N | 4.030725 | 0.198297 | -1.060472 |

2

E = -1855.29050029

| Atomic symbol | x | y | z |
|---------------|-----------|-----------|-----------|
| C | -0.463717 | 1.123064 | -0.107086 |
| P | 0.770190 | 0.128952 | 0.001655 |
| C | 2.104724 | 0.397996 | -1.252815 |
| C | 1.721685 | 1.122479 | -2.390842 |
| C | 3.434988 | -0.025754 | -1.120705 |
| C | 2.650416 | 1.389991 | -3.398729 |
| H | 0.690432 | 1.488873 | -2.439292 |
| C | 4.366898 | 0.248518 | -2.128029 |
| H | 3.753312 | -0.550561 | -0.217366 |
| C | 3.973964 | 0.949750 | -3.272047 |
| H | 2.344575 | 1.956181 | -4.281816 |
| H | 5.403661 | -0.079225 | -2.015615 |
| H | 4.702412 | 1.167236 | -4.057100 |
| C | 0.324806 | -1.650985 | -0.202601 |
| C | -0.992783 | -1.994209 | 0.140378 |
| C | 1.173379 | -2.635858 | -0.730169 |
| C | -1.448511 | -3.301957 | -0.024450 |
| H | -1.655804 | -1.208044 | 0.508084 |
| C | 0.714285 | -3.947462 | -0.899705 |

| | | | |
|---|-----------|-----------|-----------|
| H | 2.188318 | -2.373764 | -1.036310 |
| C | -0.594691 | -4.284429 | -0.543106 |
| H | -2.480548 | -3.546404 | 0.237145 |
| H | 1.379671 | -4.705864 | -1.320605 |
| H | -0.953818 | -5.307094 | -0.682306 |
| C | 1.696343 | 0.157827 | 1.604234 |
| C | 2.454842 | -0.908832 | 2.109101 |
| C | 1.543941 | 1.319886 | 2.374676 |
| C | 3.075161 | -0.805084 | 3.359158 |
| H | 2.538876 | -1.835989 | 1.537383 |
| C | 2.174290 | 1.428172 | 3.615652 |
| H | 0.894254 | 2.110627 | 1.984959 |
| C | 2.943987 | 0.367015 | 4.110064 |
| H | 3.656185 | -1.644115 | 3.750920 |
| H | 2.052907 | 2.338011 | 4.208522 |
| H | 3.426333 | 0.447425 | 5.087315 |
| S | -1.712834 | 2.129431 | -0.217168 |
| O | -1.848672 | 2.784757 | -1.537630 |
| O | -1.879600 | 3.031076 | 0.944680 |
| C | -3.092166 | 0.959303 | -0.117820 |
| C | -3.675820 | 0.662776 | 1.120620 |
| C | -3.477433 | 0.242822 | -1.259478 |
| C | -4.612730 | -0.369459 | 1.221469 |
| H | -3.364651 | 1.242706 | 1.991211 |
| C | -4.415156 | -0.785739 | -1.154924 |
| H | -3.013843 | 0.496176 | -2.214233 |
| H | -5.057976 | -0.605214 | 2.192033 |
| H | -4.702168 | -1.350902 | -2.045702 |
| H | -5.711553 | -1.912934 | 0.168143 |
| C | -4.982688 | -1.102991 | 0.086835 |

3

E = -1379.69582999

| Atomic symbol | x | y | z |
|---------------|-----------|-----------|-----------|
| C | -1.320377 | 0.104922 | -0.000001 |
| P | 0.277932 | -0.021473 | 0.000000 |
| C | 0.960228 | -0.910882 | -1.462672 |
| C | 0.050501 | -1.544978 | -2.316400 |
| C | 2.332409 | -0.984753 | -1.743783 |
| C | 0.501680 | -2.254688 | -3.431678 |
| H | -1.014491 | -1.454782 | -2.087153 |
| C | 2.786046 | -1.696276 | -2.856965 |
| H | 3.051420 | -0.469388 | -1.105176 |
| C | 1.871681 | -2.335276 | -3.700985 |
| H | -0.215878 | -2.742934 | -4.094472 |
| H | 3.855823 | -1.749244 | -3.069339 |
| H | 2.227590 | -2.889771 | -4.571554 |
| C | 0.960227 | -0.910882 | 1.462673 |
| C | 2.332407 | -0.984750 | 1.743788 |
| C | 0.050499 | -1.544982 | 2.316398 |
| C | 2.786043 | -1.696273 | 2.856970 |
| H | 3.051418 | -0.469381 | 1.105184 |
| C | 0.501678 | -2.254692 | 3.431676 |
| H | -1.014493 | -1.454788 | 2.087149 |
| C | 1.871677 | -2.335276 | 3.700986 |
| H | 3.855820 | -1.749238 | 3.069347 |
| H | -0.215881 | -2.742941 | 4.094468 |
| H | 2.227586 | -2.889772 | 4.571556 |
| C | 1.235478 | 1.553975 | 0.000001 |

| | | | |
|---|-----------|-----------|-----------|
| C | 1.515153 | 2.209720 | -1.209595 |
| C | 1.515148 | 2.209722 | 1.209598 |
| C | 2.073360 | 3.489886 | -1.209903 |
| H | 1.293218 | 1.711587 | -2.155940 |
| C | 2.073355 | 3.489887 | 1.209906 |
| H | 1.293208 | 1.711590 | 2.155942 |
| C | 2.355437 | 4.133278 | 0.000002 |
| H | 2.291876 | 3.986922 | -2.157507 |
| H | 2.291866 | 3.986925 | 2.157510 |
| H | 2.794195 | 5.132920 | 0.000002 |
| C | -4.914362 | -0.238243 | -0.000005 |
| C | -4.770654 | 1.116311 | -0.000001 |
| H | -5.811219 | -0.846222 | -0.000008 |
| H | -5.519551 | 1.899508 | 0.000001 |
| C | -2.657696 | 0.210678 | -0.000002 |
| N | -3.410285 | 1.391686 | 0.000001 |
| N | -3.640728 | -0.797293 | -0.000006 |
| C | -3.319292 | -2.204097 | -0.000010 |
| H | -2.221472 | -2.275025 | -0.000010 |
| H | -3.715463 | -2.706097 | 0.896785 |
| H | -3.715462 | -2.706091 | -0.896809 |
| C | -2.763367 | 2.683489 | 0.000006 |
| H | -2.118949 | 2.786125 | 0.887048 |
| H | -2.118949 | 2.786131 | -0.887036 |
| H | -3.527658 | 3.470391 | 0.000008 |

4

E = -1339.80438124

| Atomic symbol | x | y | z |
|---------------|-----------|-----------|-----------|
| C | -1.410925 | -0.452568 | 0.010884 |
| P | 0.134821 | -0.115953 | 0.010677 |
| C | 1.254549 | -1.446314 | -0.652173 |
| C | 0.635374 | -2.675394 | -0.913404 |
| C | 2.628491 | -1.304289 | -0.898140 |
| C | 1.376635 | -3.749046 | -1.413808 |
| H | -0.440420 | -2.746677 | -0.711702 |
| C | 3.371461 | -2.374524 | -1.409433 |
| H | 3.119902 | -0.347689 | -0.707288 |
| C | 2.747354 | -3.599878 | -1.665807 |
| H | 0.885313 | -4.705130 | -1.612679 |
| H | 4.440258 | -2.253585 | -1.607260 |
| H | 3.327974 | -4.436829 | -2.062565 |
| C | 0.869929 | 0.231272 | 1.687202 |
| C | 2.126131 | 0.815035 | 1.904081 |
| C | 0.079671 | -0.118114 | 2.788783 |
| C | 2.582299 | 1.053389 | 3.205595 |
| H | 2.742968 | 1.107632 | 1.051283 |
| C | 0.537061 | 0.104224 | 4.089855 |
| H | -0.901489 | -0.558490 | 2.579414 |
| C | 1.790421 | 0.694477 | 4.301222 |
| H | 3.557786 | 1.520915 | 3.366399 |
| H | -0.085096 | -0.176995 | 4.943719 |
| H | 2.147327 | 0.878114 | 5.317954 |
| C | 0.687981 | 1.368901 | -0.951526 |
| C | 0.997997 | 1.266921 | -2.319015 |
| C | 0.538300 | 2.653241 | -0.394246 |
| C | 1.160002 | 2.410264 | -3.105325 |
| H | 1.102429 | 0.275821 | -2.767200 |
| C | 0.696284 | 3.798338 | -1.178555 |

| | | | |
|---|-----------|-----------|-----------|
| H | 0.288095 | 2.745991 | 0.665722 |
| C | 1.009248 | 3.683561 | -2.539122 |
| H | 1.403598 | 2.310035 | -4.166584 |
| H | 0.577307 | 4.787340 | -0.727305 |
| H | 1.130982 | 4.578436 | -3.154115 |
| C | -4.737522 | -1.704690 | 0.102413 |
| C | -5.000684 | -0.368264 | -0.119330 |
| H | -5.464275 | -2.509593 | 0.211440 |
| H | -5.924027 | 0.191080 | -0.242719 |
| C | -2.765982 | -0.747657 | 0.011064 |
| N | -3.755498 | 0.242419 | -0.174117 |
| N | -3.387338 | -1.949533 | 0.179608 |
| C | -3.473145 | 1.634944 | -0.405626 |
| H | -2.399535 | 1.774930 | -0.199361 |
| H | -3.668057 | 1.931196 | -1.451936 |
| H | -4.069080 | 2.279603 | 0.262665 |

5

E = -1935.64868389

| Atomicymbol | X | Y | Z |
|-------------|------------|------------|------------|
| C | 0.2708120 | -0.0140240 | -0.5515620 |
| P | -1.2825160 | 0.0312690 | -0.1219210 |
| C | -2.4691250 | -0.3623450 | -1.4642790 |
| C | -2.0104080 | -1.1617510 | -2.5194970 |
| C | -3.7939170 | 0.0969800 | -1.4685630 |
| C | -2.8701780 | -1.5121650 | -3.5620920 |
| H | -0.9669590 | -1.4872980 | -2.5039630 |
| C | -4.6526610 | -0.2499240 | -2.5154050 |
| H | -4.1516690 | 0.7360240 | -0.6591020 |
| C | -4.1935020 | -1.0573540 | -3.5605640 |
| H | -2.5083390 | -2.1377400 | -4.3807160 |
| H | -5.6814370 | 0.1157540 | -2.5179740 |
| H | -4.8651550 | -1.3259800 | -4.3782600 |
| C | -1.8558090 | 1.6522240 | 0.5221830 |
| C | -2.8489480 | 1.7729580 | 1.5049000 |
| C | -1.2389420 | 2.8050670 | 0.0160450 |
| C | -3.2267860 | 3.0366650 | 1.9689280 |
| H | -3.3147680 | 0.8766860 | 1.9198650 |
| C | -1.6199020 | 4.0659590 | 0.4767250 |
| H | -0.4434900 | 2.6887760 | -0.7241780 |
| C | -2.6153260 | 4.1834770 | 1.4538650 |
| H | -3.9946440 | 3.1252470 | 2.7401720 |
| H | -1.1337450 | 4.9595340 | 0.0801860 |
| H | -2.9076080 | 5.1693400 | 1.8207610 |
| C | -1.7253720 | -1.1315780 | 1.2284830 |
| C | -2.7766980 | -2.0535080 | 1.1402840 |
| C | -0.9073370 | -1.1270040 | 2.3712750 |
| C | -3.0059570 | -2.9610280 | 2.1805560 |
| H | -3.4125680 | -2.0688470 | 0.2536730 |
| C | -1.1422480 | -2.0262490 | 3.4104550 |
| H | -0.0726480 | -0.4241300 | 2.4242630 |
| C | -2.1928540 | -2.9478370 | 3.3161060 |
| H | -3.8222430 | -3.6817880 | 2.1003130 |
| H | -0.5020600 | -2.0141890 | 4.2947810 |
| H | -2.3728410 | -3.6567070 | 4.1265710 |
| P | 1.8226930 | -0.0592740 | -0.9808030 |
| C | 2.7665640 | 1.3994660 | -0.4034290 |
| C | 2.2573490 | 2.1079410 | 0.6950630 |
| C | 3.9596050 | 1.8281170 | -1.0057740 |

| | | | |
|---|-----------|------------|------------|
| C | 2.9323900 | 3.2242250 | 1.1903430 |
| H | 1.3146610 | 1.7744210 | 1.1345270 |
| C | 4.6320580 | 2.9499110 | -0.5121930 |
| H | 4.3449960 | 1.2895000 | -1.8726120 |
| C | 4.1225480 | 3.6468500 | 0.5875210 |
| H | 2.5262050 | 3.7700800 | 2.0442570 |
| H | 5.5557900 | 3.2830460 | -0.9899620 |
| H | 4.6496620 | 4.5226460 | 0.9713060 |
| C | 2.7178320 | -1.5282650 | -0.3531950 |
| C | 2.0073320 | -2.4233170 | 0.4572190 |
| C | 4.0728480 | -1.7682900 | -0.6289820 |
| C | 2.6418170 | -3.5484690 | 0.9879510 |
| H | 0.9528700 | -2.2166010 | 0.6550780 |
| C | 4.7065510 | -2.8939270 | -0.0973200 |
| H | 4.6295400 | -1.0745870 | -1.2606800 |
| C | 3.9926050 | -3.7843700 | 0.7122370 |
| H | 2.0806590 | -4.2414700 | 1.6180300 |
| H | 5.7609430 | -3.0775660 | -0.3138900 |
| H | 4.4910270 | -4.6625140 | 1.1278250 |
| N | 2.3146560 | -0.1086720 | -2.6303950 |
| H | 1.8621850 | 0.6360110 | -3.1675410 |
| H | 2.0703370 | -1.0074640 | -3.0528200 |

6

E = -1935.07583925

| Atomic symbol | x | y | z |
|---------------|-----------|-----------|-----------|
| C | 0.221822 | -0.040463 | -0.707213 |
| P | -1.266290 | 0.009679 | -0.145352 |
| C | -2.557217 | -0.670642 | -1.289015 |
| C | -2.087234 | -1.128979 | -2.526065 |
| C | -3.925705 | -0.752604 | -0.996743 |
| C | -2.976369 | -1.663807 | -3.462503 |
| H | -1.009020 | -1.055221 | -2.713955 |
| C | -4.816375 | -1.290254 | -1.931293 |
| H | -4.300366 | -0.405252 | -0.031692 |
| C | -4.342250 | -1.745823 | -3.166622 |
| H | -2.602564 | -2.021657 | -4.425026 |
| H | -5.882061 | -1.355372 | -1.696547 |
| H | -5.038204 | -2.165955 | -3.897134 |
| C | -1.920200 | 1.689617 | 0.290166 |
| C | -3.030926 | 1.925463 | 1.114106 |
| C | -1.201909 | 2.780197 | -0.216620 |
| C | -3.419362 | 3.233359 | 1.421995 |
| H | -3.579292 | 1.083329 | 1.542179 |
| C | -1.592547 | 4.087330 | 0.081150 |
| H | -0.319177 | 2.563229 | -0.826462 |
| C | -2.703497 | 4.317035 | 0.902171 |
| H | -4.279387 | 3.408167 | 2.073805 |
| H | -1.021137 | 4.929465 | -0.316400 |
| H | -3.004872 | 5.338836 | 1.145690 |
| C | -1.545623 | -0.941767 | 1.407971 |
| C | -1.859027 | -2.310144 | 1.353218 |
| C | -1.178753 | -0.382505 | 2.644858 |
| C | -1.808645 | -3.099116 | 2.504897 |
| H | -2.125492 | -2.757924 | 0.393333 |
| C | -1.130164 | -1.169282 | 3.797008 |
| H | -0.915614 | 0.676735 | 2.694679 |
| C | -1.444705 | -2.532710 | 3.731841 |
| H | -2.047501 | -4.163821 | 2.444052 |

| | | | |
|---|-----------|-----------|-----------|
| H | -0.839786 | -0.719897 | 4.749990 |
| H | -1.398670 | -3.150999 | 4.631180 |
| P | 1.778242 | -0.092907 | -1.294863 |
| C | 2.641668 | 1.384930 | -0.542976 |
| C | 2.203480 | 1.967022 | 0.655024 |
| C | 3.730916 | 1.958181 | -1.214230 |
| C | 2.837644 | 3.098845 | 1.173776 |
| H | 1.336959 | 1.522905 | 1.152554 |
| C | 4.366652 | 3.094914 | -0.702949 |
| H | 4.045441 | 1.498323 | -2.155951 |
| C | 3.922234 | 3.667984 | 0.493996 |
| H | 2.480793 | 3.546997 | 2.105333 |
| H | 5.209703 | 3.539452 | -1.239924 |
| H | 4.414670 | 4.558667 | 0.893293 |
| C | 2.670757 | -1.463915 | -0.452715 |
| C | 2.214712 | -1.925985 | 0.789206 |
| C | 3.794406 | -2.063463 | -1.038457 |
| C | 2.878422 | -2.965637 | 1.446453 |
| H | 1.315658 | -1.471434 | 1.213798 |
| C | 4.457366 | -3.106796 | -0.384274 |
| H | 4.110486 | -1.708355 | -2.021631 |
| C | 4.004456 | -3.557089 | 0.861840 |
| H | 2.509036 | -3.321769 | 2.411651 |
| H | 5.328613 | -3.576679 | -0.849446 |
| H | 4.522874 | -4.373723 | 1.371572 |
| N | 2.188615 | -0.274059 | -2.835969 |
| H | 1.665163 | 0.385420 | -3.421938 |

7

E = -1484.12920448

| Atomic symbol | x | y | z |
|---------------|-----------|-----------|-----------|
| C | 1.578260 | 0.043297 | 0.141201 |
| P | -0.010213 | -0.000800 | 0.014651 |
| C | -1.007383 | 0.162934 | 1.568707 |
| C | -1.181948 | 1.432720 | 2.147278 |
| C | -1.410403 | -0.966090 | 2.301013 |
| C | -1.752031 | 1.571149 | 3.414030 |
| H | -0.853806 | 2.316020 | 1.593606 |
| C | -1.977737 | -0.831908 | 3.571302 |
| H | -1.270142 | -1.959182 | 1.867694 |
| C | -2.154231 | 0.437931 | 4.133740 |
| H | -1.883248 | 2.567147 | 3.845889 |
| H | -2.285170 | -1.722614 | 4.126255 |
| H | -2.596815 | 0.544378 | 5.127142 |
| C | -0.737054 | -1.555235 | -0.727108 |
| C | -2.102424 | -1.797659 | -0.935528 |
| C | 0.192367 | -2.527584 | -1.113289 |
| C | -2.530904 | -2.996997 | -1.516186 |
| H | -2.840972 | -1.052396 | -0.633786 |
| C | -0.229132 | -3.726999 | -1.693481 |
| H | 1.248661 | -2.294128 | -0.934358 |
| C | -1.594731 | -3.964514 | -1.896742 |
| H | -3.598024 | -3.177906 | -1.673112 |
| H | 0.506514 | -4.480487 | -1.988196 |
| H | -1.929244 | -4.900855 | -2.351159 |
| C | -0.796902 | 1.319410 | -1.048669 |
| C | -2.151549 | 1.681804 | -1.024338 |
| C | 0.071868 | 2.000580 | -1.909821 |
| C | -2.629534 | 2.705764 | -1.850660 |

| | | | |
|----|-----------|-----------|-----------|
| H | -2.834855 | 1.181945 | -0.333796 |
| C | -0.401887 | 3.012869 | -2.747227 |
| H | 1.128963 | 1.712666 | -1.873626 |
| C | -1.757036 | 3.369329 | -2.719124 |
| H | -3.685245 | 2.989233 | -1.814774 |
| H | 0.286271 | 3.534998 | -3.417731 |
| H | -2.129767 | 4.168465 | -3.365252 |
| Si | 3.320332 | 0.091659 | 0.279989 |
| C | 4.140356 | 1.444662 | -0.800840 |
| H | 3.746206 | 2.437230 | -0.529609 |
| H | 5.238672 | 1.467203 | -0.688537 |
| H | 3.910058 | 1.275422 | -1.865459 |
| C | 3.952641 | 0.427063 | 2.053692 |
| H | 3.569628 | 1.394808 | 2.414855 |
| H | 3.581416 | -0.350101 | 2.740595 |
| H | 5.054954 | 0.445839 | 2.114259 |
| C | 4.186230 | -1.533830 | -0.250371 |
| H | 3.946429 | -1.770904 | -1.299795 |
| H | 5.284973 | -1.476880 | -0.155815 |
| H | 3.832085 | -2.373295 | 0.369625 |

8

E = -1167.65583845

| Atomic symbol | x | y | z |
|---------------|-----------|-----------|-----------|
| C | 0.088821 | -0.260559 | 2.261730 |
| P | 0.023834 | -0.062600 | 0.688283 |
| C | -0.261408 | 1.648040 | 0.041959 |
| C | 0.811872 | 2.488228 | -0.298073 |
| C | -1.555811 | 2.196169 | 0.089199 |
| C | 0.597711 | 3.837243 | -0.593102 |
| H | 1.823292 | 2.076500 | -0.326462 |
| C | -1.772778 | 3.542300 | -0.208759 |
| H | -2.393982 | 1.554776 | 0.372508 |
| C | -0.696060 | 4.370500 | -0.553125 |
| H | 1.444445 | 4.476838 | -0.856248 |
| H | -2.786022 | 3.951039 | -0.171190 |
| H | -0.864304 | 5.425520 | -0.781815 |
| C | -1.313032 | -1.015237 | -0.187838 |
| C | -1.785607 | -0.725282 | -1.476636 |
| C | -1.881041 | -2.080104 | 0.522753 |
| C | -2.808488 | -1.491675 | -2.046464 |
| H | -1.372531 | 0.122402 | -2.028123 |
| C | -2.892323 | -2.855755 | -0.047827 |
| H | -1.513353 | -2.258441 | 1.538858 |
| C | -3.359633 | -2.562651 | -1.336236 |
| H | -3.179032 | -1.250497 | -3.046565 |
| H | -3.326389 | -3.686320 | 0.514811 |
| H | -4.157994 | -3.161915 | -1.781205 |
| C | 1.554199 | -0.575741 | -0.237741 |
| C | 1.692352 | -0.543766 | -1.633396 |
| C | 2.614785 | -1.049756 | 0.543170 |
| C | 2.879326 | -0.972173 | -2.237709 |
| H | 0.874047 | -0.174555 | -2.254390 |
| C | 3.802545 | -1.476870 | -0.056478 |
| H | 2.465485 | -1.068299 | 1.628271 |
| C | 3.937262 | -1.438729 | -1.450341 |
| H | 2.979691 | -0.942840 | -3.326117 |
| H | 4.626276 | -1.841444 | 0.562676 |
| H | 4.864097 | -1.774209 | -1.922596 |

| | | | |
|---|----------|-----------|----------|
| C | 0.143827 | -0.428115 | 3.593528 |
| N | 0.197093 | -0.592281 | 4.774523 |

9

E = -2111.40225977

| Atomic symbols | X | Y | Z |
|----------------|------------|------------|------------|
| C | -0.0006780 | 0.0001090 | 0.0000170 |
| P | 1.6088950 | 0.0001640 | 0.0003330 |
| P | -1.6102470 | 0.0000540 | -0.0002990 |
| C | 2.3670390 | 1.5258430 | -0.6821590 |
| C | 2.3679470 | -1.3532420 | -0.9796480 |
| C | -2.3689360 | -0.2982210 | 1.6441010 |
| C | 2.3679000 | -0.1719700 | 1.6624010 |
| C | -2.3680270 | -1.2754890 | -1.0804880 |
| C | -2.3683060 | 1.5734620 | -0.5643780 |
| C | 1.6575080 | 2.1971710 | -1.6890630 |
| C | 2.1654650 | 3.3730220 | -2.2423660 |
| C | 3.3834770 | 3.8923920 | -1.7879790 |
| C | 4.0892810 | 3.2327860 | -0.7777900 |
| C | 1.6587220 | -2.5610770 | -1.0578810 |
| C | 2.1674620 | -3.6282440 | -1.7988190 |
| C | 3.5838720 | 2.0515760 | -0.2254070 |
| C | 3.3859140 | -3.4943370 | -2.4750380 |
| C | 4.0912700 | -2.2894520 | -2.4088460 |
| C | 3.5851130 | -1.2204420 | -1.6625250 |
| C | -1.6633660 | -1.1215510 | 2.5343290 |
| C | -2.1721570 | -1.3785940 | 3.8077710 |
| C | -3.3869060 | -0.8077120 | 4.2055610 |
| C | -4.0884980 | 0.0218880 | 3.3262220 |
| C | -3.5823150 | 0.2766380 | 2.0476060 |
| C | 1.6560790 | 0.3583400 | 2.7487550 |
| C | 2.1659590 | 0.2505040 | 4.0430540 |
| C | 3.3878570 | -0.3961790 | 4.2633920 |
| C | 4.0955070 | -0.9360350 | 3.1856920 |
| C | 3.5882830 | -0.8245990 | 1.8872030 |
| C | -1.6569410 | -1.6416240 | -2.2329900 |
| C | -2.1644660 | -2.6169370 | -3.0920120 |
| C | -3.3833910 | -3.2411070 | -2.8015790 |
| C | -4.0903280 | -2.8878230 | -1.6486720 |
| C | -3.5854330 | -1.9068170 | -0.7891980 |
| C | -3.5826820 | 1.6365780 | -1.2622980 |
| C | -4.0874870 | 2.8716410 | -1.6814440 |
| C | -3.3838650 | 4.0471820 | -1.4045810 |
| C | -2.1683110 | 3.9871010 | -0.7127710 |
| C | -1.6606750 | 2.7553340 | -0.2984420 |
| H | -0.6992200 | 2.6844740 | 0.2157450 |
| H | -1.6111150 | 4.9024320 | -0.5034900 |
| H | -3.7776690 | 5.0100980 | -1.7357970 |
| H | -5.0293550 | 2.9144320 | -2.2322120 |
| H | -4.1261350 | 0.7183910 | -1.4938390 |
| H | -0.7025590 | -1.5330900 | 2.2160460 |
| H | -1.6164940 | -2.0190720 | 4.4956110 |
| H | -3.7816640 | -1.0025550 | 5.2046550 |
| H | -5.0298880 | 0.4786760 | 3.6383420 |
| H | -4.1238310 | 0.9375490 | 1.3680520 |
| H | -0.6929870 | -1.1649740 | -2.4256700 |
| H | -1.6044960 | -2.8977480 | -3.9862750 |
| H | -3.7771480 | -4.0097450 | -3.4695180 |
| H | -5.0348270 | -3.3823590 | -1.4127850 |

| | | | |
|---|------------|------------|------------|
| H | -4.1308220 | -1.6443670 | 0.1194070 |
| H | 4.1288520 | 1.5469430 | 0.5747800 |
| H | 5.0332790 | 3.6424090 | -0.4125930 |
| H | 3.7776250 | 4.8164510 | -2.2154810 |
| H | 1.6065570 | 3.8909740 | -3.0243170 |
| H | 0.6945930 | 1.7916390 | -2.0086830 |
| H | 1.6089540 | -4.5646600 | -1.8563470 |
| H | 0.6954240 | -2.6353270 | -0.5479650 |
| H | 4.1296340 | -0.2749370 | -1.6251670 |
| H | 5.0355720 | -2.1778420 | -2.9456240 |
| H | 3.7807030 | -4.3267160 | -3.0609330 |
| H | 0.6899280 | 0.8321100 | 2.5591520 |
| H | 4.1347720 | -1.2613670 | 1.0489960 |
| H | 5.0423290 | -1.4524840 | 3.3562740 |
| H | 3.7834290 | -0.4873790 | 5.2769010 |
| H | 1.6054890 | 0.6640780 | 4.8838530 |

1.3 BP86-D3(BJ)/Def2TZVP, 150° structures

1

E = -1871.86129184

| Atomic symbol | x | y | z |
|---------------|-----------|-----------|-----------|
| C | -0.207947 | -0.383098 | -1.492472 |
| P | 0.750940 | -0.027932 | -0.211013 |
| C | 1.453993 | -1.410383 | 0.764776 |
| C | 0.917482 | -2.685292 | 0.528485 |
| C | 2.468411 | -1.242807 | 1.720928 |
| C | 1.385855 | -3.780789 | 1.260920 |
| H | 0.151552 | -2.814646 | -0.243321 |
| C | 2.929359 | -2.340213 | 2.449745 |
| H | 2.903821 | -0.257213 | 1.893697 |
| C | 2.385689 | -3.610082 | 2.222183 |
| H | 0.971265 | -4.772517 | 1.070267 |
| H | 3.718926 | -2.207475 | 3.192081 |
| H | 2.751747 | -4.468104 | 2.789548 |
| C | -0.145410 | 0.995074 | 1.005356 |
| C | -0.569740 | 2.276119 | 0.607087 |
| C | -0.521212 | 0.503377 | 2.264247 |
| C | -1.333677 | 3.061386 | 1.470030 |
| H | -0.288004 | 2.648237 | -0.379642 |
| C | -1.292734 | 1.291226 | 3.123960 |
| H | -0.194928 | -0.490626 | 2.573741 |
| C | -1.698764 | 2.570260 | 2.730463 |
| H | -1.639536 | 4.063793 | 1.163463 |
| H | -1.566588 | 0.908298 | 4.109360 |
| H | -2.280738 | 3.193800 | 3.412763 |
| C | 2.174352 | 0.988515 | -0.721161 |
| C | 2.831792 | 1.849460 | 0.169356 |
| C | 2.612393 | 0.883522 | -2.047487 |
| C | 3.934695 | 2.590025 | -0.263836 |
| H | 2.467250 | 1.961885 | 1.192750 |
| C | 3.719857 | 1.618126 | -2.474049 |
| H | 2.054476 | 0.240102 | -2.733013 |
| C | 4.382845 | 2.469441 | -1.582830 |
| H | 4.440135 | 3.267757 | 0.426840 |
| H | 4.061348 | 1.534413 | -3.507414 |
| H | 5.243720 | 3.049684 | -1.920473 |
| S | -1.384910 | -1.283101 | -2.165200 |

| | | | |
|---|-----------|-----------|-----------|
| O | -1.380380 | -2.726853 | -1.867462 |
| O | -1.700623 | -0.905484 | -3.542755 |
| C | -2.541861 | -0.509053 | -1.076033 |
| C | -3.068296 | 0.777701 | -1.372817 |
| C | -2.838011 | -1.089370 | 0.186780 |
| C | -3.749987 | 1.466190 | -0.408180 |
| H | -2.896259 | 1.210938 | -2.357011 |
| C | -3.525635 | -0.363652 | 1.120151 |
| H | -2.490906 | -2.097851 | 0.406976 |
| H | -4.154442 | 2.466420 | -0.551460 |
| H | -3.764027 | -0.732696 | 2.115755 |
| H | -4.404417 | 1.452411 | 1.552702 |
| N | -3.966084 | 0.899511 | 0.824129 |

2

E = -1855.29868999

| Atomic symbol | x | y | z |
|---------------|-----------|-----------|-----------|
| C | -0.120654 | -0.102820 | -1.540822 |
| P | 0.820422 | 0.042903 | -0.251623 |
| C | 1.791092 | -1.458983 | 0.231055 |
| C | 1.308398 | -2.666299 | -0.297855 |
| C | 2.932595 | -1.466682 | 1.045761 |
| C | 1.950155 | -3.869427 | 0.009595 |
| H | 0.437833 | -2.634151 | -0.965014 |
| C | 3.579132 | -2.670830 | 1.343078 |
| H | 3.323069 | -0.528904 | 1.446379 |
| C | 3.084772 | -3.874770 | 0.829517 |
| H | 1.566638 | -4.806661 | -0.400789 |
| H | 4.471512 | -2.670290 | 1.974545 |
| H | 3.590159 | -4.815658 | 1.061423 |
| C | -0.037454 | 0.501812 | 1.310855 |
| C | -0.840386 | 1.656877 | 1.271621 |
| C | -0.103981 | -0.333439 | 2.435487 |
| C | -1.680844 | 1.970693 | 2.337000 |
| H | -0.826484 | 2.277844 | 0.373308 |
| C | -0.946409 | -0.015307 | 3.505819 |
| H | 0.495691 | -1.245143 | 2.465238 |
| C | -1.735690 | 1.136772 | 3.460494 |
| H | -2.318883 | 2.855056 | 2.281093 |
| H | -0.995270 | -0.678620 | 4.373234 |
| H | -2.407581 | 1.375545 | 4.288011 |
| C | 2.089948 | 1.355520 | -0.448969 |
| C | 2.703235 | 1.990670 | 0.639975 |
| C | 2.414480 | 1.748079 | -1.753591 |
| C | 3.646731 | 3.001520 | 0.424557 |
| H | 2.418901 | 1.713460 | 1.658109 |
| C | 3.365991 | 2.746387 | -1.968664 |
| H | 1.871737 | 1.264697 | -2.572779 |
| C | 3.985248 | 3.374924 | -0.879435 |
| H | 4.111980 | 3.504293 | 1.276247 |
| H | 3.619010 | 3.047371 | -2.988288 |
| H | 4.720549 | 4.165589 | -1.048055 |
| S | -1.465366 | -0.677056 | -2.238764 |
| O | -1.510821 | -2.157474 | -2.345121 |
| O | -1.836076 | 0.043516 | -3.471497 |
| C | -2.735679 | -0.249891 | -1.020374 |
| C | -3.494191 | 0.917111 | -1.165459 |
| C | -2.878318 | -1.035085 | 0.132395 |
| C | -4.389272 | 1.297495 | -0.160742 |

| | | | |
|---|-----------|-----------|-----------|
| H | -3.364369 | 1.508185 | -2.073746 |
| C | -3.768740 | -0.649880 | 1.134026 |
| H | -2.276976 | -1.940567 | 0.228328 |
| H | -4.979807 | 2.210678 | -0.277184 |
| H | -3.861731 | -1.255337 | 2.038809 |
| H | -5.220929 | 0.821561 | 1.782381 |
| C | -4.530215 | 0.517567 | 0.992386 |

3

E= -1379.70190012

| Atomic symbol | x | y | z |
|---------------|-----------|-----------|-----------|
| C | -1.281724 | -0.643975 | -0.000001 |
| P | 0.267174 | -0.140280 | 0.000000 |
| C | 1.185469 | -0.790562 | -1.455501 |
| C | 0.525685 | -1.700478 | -2.289441 |
| C | 2.506289 | -0.419783 | -1.748665 |
| C | 1.175926 | -2.237796 | -3.402718 |
| H | -0.505031 | -1.964016 | -2.036284 |
| C | 3.157362 | -0.956608 | -2.861624 |
| H | 3.025258 | 0.305205 | -1.119667 |
| C | 2.493992 | -1.868381 | -3.689508 |
| H | 0.653345 | -2.945518 | -4.049743 |
| H | 4.184294 | -0.660717 | -3.085533 |
| H | 3.004115 | -2.287211 | -4.559274 |
| C | 1.185466 | -0.790563 | 1.455503 |
| C | 2.506287 | -0.419785 | 1.748669 |
| C | 0.525682 | -1.700481 | 2.289440 |
| C | 3.157358 | -0.956612 | 2.861628 |
| H | 3.025257 | 0.305203 | 1.119672 |
| C | 1.175921 | -2.237799 | 3.402717 |
| H | -0.505035 | -1.964018 | 2.036281 |
| C | 2.493987 | -1.868385 | 3.689510 |
| H | 4.184290 | -0.660721 | 3.085538 |
| H | 0.653339 | -2.945522 | 4.049741 |
| H | 3.004108 | -2.287216 | 4.559276 |
| C | 0.729090 | 1.646163 | 0.000001 |
| C | 0.801594 | 2.356897 | -1.209687 |
| C | 0.801594 | 2.356896 | 1.209691 |
| C | 0.953963 | 3.745285 | -1.209904 |
| H | 0.740609 | 1.815285 | -2.156210 |
| C | 0.953963 | 3.745284 | 1.209910 |
| H | 0.740609 | 1.815282 | 2.156213 |
| C | 1.030000 | 4.443784 | 0.000003 |
| H | 1.015724 | 4.284434 | -2.157557 |
| H | 1.015724 | 4.284431 | 2.157563 |
| H | 1.151460 | 5.528610 | 0.000004 |
| C | -4.884599 | -0.682050 | -0.000005 |
| C | -4.664162 | 0.660327 | -0.000003 |
| H | -5.813398 | -1.239823 | -0.000006 |
| H | -5.363634 | 1.487834 | -0.000003 |
| C | -2.605596 | -0.362922 | -0.000002 |
| N | -3.287456 | 0.859589 | -0.000002 |
| N | -3.645141 | -1.309897 | -0.000004 |
| C | -3.401704 | -2.733147 | -0.000005 |
| H | -2.308379 | -2.857985 | -0.000004 |
| H | -3.825549 | -3.210671 | 0.897445 |
| H | -3.825547 | -3.210669 | -0.897457 |
| C | -2.601153 | 2.128666 | 0.000001 |
| H | -1.956328 | 2.221723 | 0.887124 |

| | | | |
|---|-----------|----------|-----------|
| H | -1.956327 | 2.221725 | -0.887121 |
| H | -3.342458 | 2.936864 | 0.000001 |

4

E= -1339.80978854

| Atomic symbol | x | y | z |
|---------------|-----------|-----------|-----------|
| C | -1.403617 | 0.469349 | -0.268600 |
| P | 0.133559 | 0.054983 | -0.065004 |
| C | 0.679260 | -1.638146 | -0.620736 |
| C | -0.362359 | -2.553711 | -0.847925 |
| C | 2.004656 | -2.033770 | -0.866176 |
| C | -0.074744 | -3.848119 | -1.291617 |
| H | -1.398149 | -2.230642 | -0.672338 |
| C | 2.288124 | -3.323897 | -1.326906 |
| H | 2.823362 | -1.331398 | -0.699441 |
| C | 1.248780 | -4.236738 | -1.535810 |
| H | -0.891603 | -4.556422 | -1.453540 |
| H | 3.323160 | -3.618905 | -1.521886 |
| H | 1.470132 | -5.246148 | -1.892666 |
| C | 0.823458 | 0.123687 | 1.651699 |
| C | 0.983624 | 1.376638 | 2.275410 |
| C | 0.971584 | -1.036092 | 2.433177 |
| C | 1.298728 | 1.466614 | 3.630815 |
| H | 0.849778 | 2.283457 | 1.679641 |
| C | 1.277094 | -0.947499 | 3.793688 |
| H | 0.841950 | -2.014081 | 1.964139 |
| C | 1.446739 | 0.303063 | 4.400605 |
| H | 1.431163 | 2.448114 | 4.094705 |
| H | 1.388142 | -1.860675 | 4.385012 |
| H | 1.686601 | 0.372408 | 5.464302 |
| C | 1.268414 | 1.203215 | -0.963548 |
| C | 2.630550 | 1.338896 | -0.659042 |
| C | 0.722710 | 1.959711 | -2.007177 |
| C | 3.436220 | 2.218941 | -1.391763 |
| H | 3.054893 | 0.777360 | 0.176764 |
| C | 1.524601 | 2.830539 | -2.746569 |
| H | -0.352622 | 1.843596 | -2.186103 |
| C | 2.887064 | 2.962458 | -2.440271 |
| H | 4.494439 | 2.328572 | -1.139371 |
| H | 1.089843 | 3.416275 | -3.561148 |
| H | 3.515963 | 3.648648 | -3.013516 |
| C | -4.728577 | -0.827246 | -0.223518 |
| C | -4.995635 | 0.526124 | -0.172680 |
| H | -5.452472 | -1.641707 | -0.241218 |
| H | -5.921642 | 1.093042 | -0.136631 |
| C | -2.755788 | 0.145871 | -0.216509 |
| N | -3.753169 | 1.142972 | -0.166171 |
| N | -3.378468 | -1.071447 | -0.247262 |
| C | -3.481786 | 2.555939 | -0.117180 |
| H | -2.382265 | 2.647260 | -0.110971 |
| H | -3.891080 | 3.081826 | -0.998400 |
| H | -3.896113 | 3.019038 | 0.795574 |

5

E= -1935.65181984

| Atomic symbol | x | y | z |
|---------------|-----------|-----------|-----------|
| C | 0.277654 | 0.662601 | -0.368067 |
| P | -1.262790 | 0.241783 | -0.071651 |
| C | -1.965433 | -1.083086 | -1.132935 |

| | | | |
|---|-----------|-----------|-----------|
| C | -1.254793 | -2.295563 | -1.188075 |
| C | -3.097470 | -0.914024 | -1.940735 |
| C | -1.679162 | -3.323420 | -2.028819 |
| H | -0.359396 | -2.422867 | -0.574508 |
| C | -3.514475 | -1.942772 | -2.793290 |
| H | -3.651286 | 0.025595 | -1.909622 |
| C | -2.810478 | -3.148076 | -2.836638 |
| H | -1.124294 | -4.263303 | -2.058804 |
| H | -4.393296 | -1.799257 | -3.425296 |
| H | -3.138419 | -3.950384 | -3.500357 |
| C | -2.428447 | 1.642358 | -0.238819 |
| C | -3.721731 | 1.611910 | 0.303092 |
| C | -1.992781 | 2.774528 | -0.937095 |
| C | -4.576550 | 2.703511 | 0.132861 |
| H | -4.057027 | 0.739457 | 0.867746 |
| C | -2.849138 | 3.864737 | -1.108005 |
| H | -0.968221 | 2.774971 | -1.319843 |
| C | -4.142120 | 3.829175 | -0.575459 |
| H | -5.581217 | 2.679641 | 0.559587 |
| H | -2.506280 | 4.747055 | -1.652343 |
| H | -4.810178 | 4.683123 | -0.704072 |
| C | -1.574576 | -0.374749 | 1.630125 |
| C | -2.506726 | -1.380842 | 1.919209 |
| C | -0.814612 | 0.182797 | 2.669780 |
| C | -2.675396 | -1.825200 | 3.234743 |
| H | -3.088485 | -1.830586 | 1.112377 |
| C | -0.988289 | -0.257068 | 3.982137 |
| H | -0.071376 | 0.945347 | 2.423477 |
| C | -1.919270 | -1.263556 | 4.266824 |
| H | -3.395081 | -2.617124 | 3.451930 |
| H | -0.392704 | 0.180463 | 4.785863 |
| H | -2.049397 | -1.613693 | 5.292645 |
| P | 1.771438 | 0.267714 | -0.859636 |
| C | 2.997392 | 1.522829 | -0.357460 |
| C | 2.566563 | 2.583044 | 0.449672 |
| C | 4.347602 | 1.434907 | -0.729472 |
| C | 3.475674 | 3.552039 | 0.879802 |
| H | 1.506203 | 2.619974 | 0.715185 |
| C | 5.255784 | 2.403664 | -0.296601 |
| H | 4.683183 | 0.610476 | -1.360313 |
| C | 4.821389 | 3.462257 | 0.508684 |
| H | 3.135082 | 4.378906 | 1.506453 |
| H | 6.305902 | 2.333271 | -0.587263 |
| H | 5.533671 | 4.217570 | 0.846908 |
| C | 2.406024 | -1.338108 | -0.237151 |
| C | 1.868971 | -1.823313 | 0.965608 |
| C | 3.370435 | -2.100384 | -0.914476 |
| C | 2.288336 | -3.048683 | 1.484635 |
| H | 1.105931 | -1.233966 | 1.478031 |
| C | 3.782262 | -3.333144 | -0.398582 |
| H | 3.782497 | -1.728463 | -1.853579 |
| C | 3.244858 | -3.808226 | 0.801152 |
| H | 1.862313 | -3.414771 | 2.420810 |
| H | 4.524669 | -3.925833 | -0.937264 |
| H | 3.568263 | -4.770938 | 1.201985 |
| N | 2.171988 | 0.107370 | -2.529692 |
| H | 2.037767 | 1.002357 | -3.007645 |
| H | 1.558574 | -0.581930 | -2.974811 |

6

E = -1935.08236308

| Atomic symbol | x | y | z |
|---------------|-----------|-----------|-----------|
| C | 0.246362 | 0.600412 | -0.774076 |
| P | -1.203638 | 0.320481 | -0.149910 |
| C | -2.413228 | -0.529653 | -1.275255 |
| C | -1.864677 | -1.055221 | -2.453780 |
| C | -3.783234 | -0.687616 | -1.022144 |
| C | -2.676825 | -1.741477 | -3.361548 |
| H | -0.790803 | -0.913805 | -2.632813 |
| C | -4.597662 | -1.364748 | -1.935196 |
| H | -4.220275 | -0.282815 | -0.107234 |
| C | -4.044239 | -1.895329 | -3.105976 |
| H | -2.239113 | -2.157210 | -4.272489 |
| H | -5.665722 | -1.481506 | -1.733073 |
| H | -4.680173 | -2.427108 | -3.818328 |
| C | -2.088354 | 1.841960 | 0.390112 |
| C | -3.162311 | 1.843250 | 1.292440 |
| C | -1.626297 | 3.058438 | -0.128797 |
| C | -3.766401 | 3.047637 | 1.669871 |
| H | -3.507990 | 0.902010 | 1.725617 |
| C | -2.237222 | 4.259616 | 0.235436 |
| H | -0.764973 | 3.015493 | -0.804376 |
| C | -3.309125 | 4.257161 | 1.138131 |
| H | -4.593099 | 3.042080 | 2.384878 |
| H | -1.872382 | 5.203819 | -0.176614 |
| H | -3.781138 | 5.197614 | 1.433026 |
| C | -1.233612 | -0.762763 | 1.338723 |
| C | -1.275657 | -2.157746 | 1.174790 |
| C | -0.917245 | -0.241490 | 2.605031 |
| C | -1.020576 | -3.008563 | 2.251242 |
| H | -1.484572 | -2.574067 | 0.187271 |
| C | -0.677733 | -1.092271 | 3.685812 |
| H | -0.844528 | 0.841073 | 2.734717 |
| C | -0.730005 | -2.480696 | 3.513275 |
| H | -1.029899 | -4.090211 | 2.099810 |
| H | -0.436546 | -0.671444 | 4.665425 |
| H | -0.522678 | -3.147294 | 4.353390 |
| P | 1.718936 | 0.033380 | -1.326715 |
| C | 2.978141 | 1.279970 | -0.774534 |
| C | 2.644252 | 2.320062 | 0.102404 |
| C | 4.293380 | 1.189824 | -1.254946 |
| C | 3.606429 | 3.256317 | 0.496314 |
| H | 1.607535 | 2.367786 | 0.450790 |
| C | 5.259802 | 2.118019 | -0.858200 |
| H | 4.531074 | 0.389164 | -1.960653 |
| C | 4.918367 | 3.154971 | 0.019923 |
| H | 3.334529 | 4.067192 | 1.178207 |
| H | 6.283096 | 2.039167 | -1.236172 |
| H | 5.672672 | 3.884385 | 0.327061 |
| C | 2.164533 | -1.418504 | -0.290087 |
| C | 2.232550 | -1.294410 | 1.106812 |
| C | 2.285866 | -2.689818 | -0.867898 |
| C | 2.415774 | -2.418479 | 1.911841 |
| H | 2.111913 | -0.307795 | 1.559455 |
| C | 2.461226 | -3.819015 | -0.060526 |
| H | 2.228349 | -2.756496 | -1.956947 |
| C | 2.527840 | -3.687727 | 1.330816 |
| H | 2.445389 | -2.309430 | 2.998398 |

| | | | |
|---|----------|-----------|-----------|
| H | 2.547232 | -4.808353 | -0.519278 |
| H | 2.656493 | -4.570686 | 1.962215 |
| N | 1.997251 | -0.467969 | -2.827810 |
| H | 1.644660 | 0.223664 | -3.498295 |

7

E= -1484.13189564

| Atomic symbol | x | y | z |
|---------------|-----------|-----------|-----------|
| C | 1.305226 | -0.189516 | -0.988402 |
| P | -0.087616 | -0.031111 | -0.206588 |
| C | -0.105670 | -0.217714 | 1.633855 |
| C | 0.308947 | 0.856467 | 2.442789 |
| C | -0.257797 | -1.481961 | 2.230099 |
| C | 0.555778 | 0.675322 | 3.804636 |
| H | 0.450305 | 1.839556 | 1.986809 |
| C | -0.010718 | -1.666515 | 3.592652 |
| H | -0.564360 | -2.328279 | 1.610699 |
| C | 0.397422 | -0.588710 | 4.388162 |
| H | 0.878027 | 1.522533 | 4.416222 |
| H | -0.134002 | -2.657704 | 4.037833 |
| H | 0.595958 | -0.733156 | 5.452840 |
| C | -1.403675 | -1.236978 | -0.732737 |
| C | -2.684044 | -1.330053 | -0.168956 |
| C | -1.048435 | -2.110137 | -1.767089 |
| C | -3.593020 | -2.290524 | -0.627349 |
| H | -2.971363 | -0.660898 | 0.644551 |
| C | -1.955595 | -3.064431 | -2.234944 |
| H | -0.032510 | -1.999310 | -2.167647 |
| C | -3.231404 | -3.158398 | -1.663311 |
| H | -4.586320 | -2.362700 | -0.175687 |
| H | -1.669038 | -3.742033 | -3.044077 |
| H | -3.942241 | -3.907071 | -2.023052 |
| C | -0.969217 | 1.601693 | -0.417224 |
| C | -2.024295 | 2.064588 | 0.382804 |
| C | -0.483085 | 2.423733 | -1.441343 |
| C | -2.582984 | 3.328768 | 0.162090 |
| H | -2.393794 | 1.447216 | 1.204847 |
| C | -1.048333 | 3.678974 | -1.677137 |
| H | 0.364655 | 2.037481 | -2.020355 |
| C | -2.100896 | 4.136522 | -0.873069 |
| H | -3.394831 | 3.686707 | 0.801550 |
| H | -0.662301 | 4.310585 | -2.482069 |
| H | -2.538061 | 5.123303 | -1.046820 |
| Si | 3.063143 | -0.223466 | -0.975916 |
| C | 3.868179 | 1.384734 | -1.634717 |
| H | 3.574811 | 2.239648 | -1.004348 |
| H | 4.970969 | 1.331194 | -1.653135 |
| H | 3.518382 | 1.594174 | -2.658790 |
| C | 3.831208 | -0.503185 | 0.753119 |
| H | 3.513781 | 0.295692 | 1.441974 |
| H | 3.473070 | -1.455375 | 1.175391 |
| H | 4.934968 | -0.525535 | 0.732997 |
| C | 3.781403 | -1.607749 | -2.084237 |
| H | 3.423687 | -1.489852 | -3.120039 |
| H | 4.885322 | -1.607470 | -2.099117 |
| H | 3.441161 | -2.593095 | -1.727074 |

8

E= -1167.65886820

| Atomic symbol | x | y | z |
|---------------|-----------|-----------|-----------|
| C | -0.029737 | -0.115792 | 2.303796 |
| P | 0.001075 | -0.028148 | 0.698236 |
| C | -0.242728 | 1.601712 | -0.144681 |
| C | 0.845516 | 2.446471 | -0.426189 |
| C | -1.544771 | 2.117537 | -0.284920 |
| C | 0.639590 | 3.760009 | -0.854322 |
| H | 1.861871 | 2.064850 | -0.304751 |
| C | -1.752363 | 3.429438 | -0.712379 |
| H | -2.399091 | 1.479508 | -0.045763 |
| C | -0.660454 | 4.258193 | -1.003106 |
| H | 1.498303 | 4.400219 | -1.073758 |
| H | -2.771278 | 3.811313 | -0.817357 |
| H | -0.822265 | 5.286556 | -1.334431 |
| C | -1.201879 | -1.099217 | -0.247314 |
| C | -1.568312 | -0.911523 | -1.589123 |
| C | -1.792294 | -2.142896 | 0.478026 |
| C | -2.504624 | -1.755743 | -2.195176 |
| H | -1.137736 | -0.083809 | -2.157487 |
| C | -2.719559 | -2.994214 | -0.126601 |
| H | -1.512617 | -2.247039 | 1.531533 |
| C | -3.078259 | -2.803281 | -1.467151 |
| H | -2.790257 | -1.594506 | -3.238361 |
| H | -3.173432 | -3.804165 | 0.450268 |
| H | -3.810050 | -3.462939 | -1.940177 |
| C | 1.630904 | -0.586720 | 0.045628 |
| C | 1.919713 | -0.673859 | -1.324149 |
| C | 2.609294 | -0.946691 | 0.979037 |
| C | 3.180130 | -1.103750 | -1.753905 |
| H | 1.161588 | -0.397817 | -2.059471 |
| C | 3.867057 | -1.379066 | 0.552496 |
| H | 2.328251 | -0.867540 | 2.035867 |
| C | 4.156476 | -1.456584 | -0.816992 |
| H | 3.400091 | -1.165637 | -2.822930 |
| H | 4.627010 | -1.656734 | 1.287598 |
| H | 5.140258 | -1.794299 | -1.152975 |
| C | -0.662636 | 0.111994 | 3.477868 |
| N | -1.166165 | 0.274021 | 4.546228 |

9

E = -2111.40693928

| Atomic symbol | x | y | z |
|---------------|-----------|-----------|-----------|
| C | 0.000000 | -0.000002 | 0.705027 |
| P | -1.564429 | 0.077249 | 0.285329 |
| P | 1.564429 | -0.077251 | 0.285329 |
| C | -2.028270 | 1.562514 | -0.686315 |
| C | -2.687110 | 0.039845 | 1.725984 |
| C | 2.028272 | -1.562514 | -0.686319 |
| C | -2.113314 | -1.321210 | -0.765113 |
| C | 2.687111 | -0.039849 | 1.725984 |
| C | 2.113312 | 1.321211 | -0.765110 |
| C | -1.190380 | 2.681669 | -0.581197 |
| C | -1.445603 | 3.824739 | -1.339473 |
| C | -2.540230 | 3.857524 | -2.209967 |
| C | -3.377503 | 2.742685 | -2.322254 |
| C | -2.158522 | -0.371404 | 2.955778 |
| C | -2.980865 | -0.446172 | 4.082342 |
| C | -3.121867 | 1.596464 | -1.564674 |
| C | -4.333707 | -0.104425 | 3.984503 |

| | | | |
|---|-----------|-----------|-----------|
| C | -4.863046 | 0.312749 | 2.758468 |
| C | -4.042832 | 0.383921 | 1.630118 |
| C | 1.190389 | -2.681673 | -0.581198 |
| C | 1.445613 | -3.824741 | -1.339476 |
| C | 2.540236 | -3.857521 | -2.209975 |
| C | 3.377503 | -2.742678 | -2.322265 |
| C | 3.121866 | -1.596459 | -1.564683 |
| C | -1.644880 | -1.377332 | -2.088984 |
| C | -1.836995 | -2.522944 | -2.859063 |
| C | -2.494970 | -3.631877 | -2.313339 |
| C | -2.965229 | -3.583105 | -0.998131 |
| C | -2.778096 | -2.431790 | -0.226534 |
| C | 2.158522 | 0.371398 | 2.955778 |
| C | 2.980866 | 0.446165 | 4.082342 |
| C | 4.333708 | 0.104420 | 3.984502 |
| C | 4.863047 | -0.312752 | 2.758467 |
| C | 4.042833 | -0.383922 | 1.630117 |
| C | 2.778093 | 2.431789 | -0.226529 |
| C | 2.965225 | 3.583108 | -0.998123 |
| C | 2.494962 | 3.631883 | -2.313329 |
| C | 1.836987 | 2.522953 | -2.859055 |
| C | 1.644875 | 1.377338 | -2.088980 |
| H | 1.113074 | 0.519366 | -2.506067 |
| H | 1.463298 | 2.557889 | -3.884131 |
| H | 2.639024 | 4.532182 | -2.913581 |
| H | 3.481217 | 4.444647 | -0.569310 |
| H | 3.139573 | 2.398193 | 0.803047 |
| H | 0.324519 | -2.624944 | 0.081887 |
| H | 0.778413 | -4.685162 | -1.261987 |
| H | 2.736076 | -4.748640 | -2.809744 |
| H | 4.225496 | -2.762007 | -3.009932 |
| H | 3.757495 | -0.715690 | -1.678497 |
| H | 1.095490 | 0.623783 | 2.995902 |
| H | 2.565923 | 0.768957 | 5.039366 |
| H | 4.976495 | 0.158177 | 4.865398 |
| H | 5.917014 | -0.587273 | 2.682760 |
| H | 4.457248 | -0.717148 | 0.676983 |
| H | -3.757502 | 0.715699 | -1.678485 |
| H | -4.225499 | 2.762018 | -3.009917 |
| H | -2.736069 | 4.748645 | -2.809735 |
| H | -0.778399 | 4.685156 | -1.261988 |
| H | -0.324508 | 2.624935 | 0.081883 |
| H | -2.565923 | -0.768966 | 5.039365 |
| H | -1.095491 | -0.623790 | 2.995902 |
| H | -4.457247 | 0.717148 | 0.676984 |
| H | -5.917013 | 0.587272 | 2.682761 |
| H | -4.976495 | -0.158183 | 4.865398 |
| H | -1.113080 | -0.519359 | -2.506069 |
| H | -3.139574 | -2.398197 | 0.803042 |
| H | -3.481221 | -4.444646 | -0.569321 |
| H | -2.639033 | -4.532173 | -2.913594 |
| H | -1.463308 | -2.557878 | -3.884140 |

1.4 BP86-D3(BJ)/Def2TZVP, Dissociation structures

L1

E = -797.120965110

| Atomic symbol | x | y | z |
|---------------|----------|----------|-----------|
| S | 1.700228 | 0.000003 | -0.271940 |

| | | | |
|---|-----------|-----------|-----------|
| O | 2.291402 | 1.285772 | 0.185362 |
| O | 2.291393 | -1.285780 | 0.185338 |
| C | -0.025434 | -0.000001 | 0.120646 |
| C | -0.753358 | -1.221704 | 0.071846 |
| C | -0.753356 | 1.221703 | 0.071837 |
| C | -2.119328 | -1.200789 | -0.003012 |
| H | -0.214912 | -2.168539 | 0.124322 |
| C | -2.119327 | 1.200790 | -0.003022 |
| H | -0.214909 | 2.168538 | 0.124305 |
| H | -2.739914 | -2.095662 | 0.007837 |
| H | -2.739903 | 2.095671 | 0.007816 |
| H | -3.803448 | 0.000000 | -0.092866 |
| N | -2.789727 | 0.000003 | -0.047965 |

L1+

E= -796.867899594

| Atomic symbol | x | y | z |
|---------------|-----------|-----------|-----------|
| S | 1.762317 | 0.000001 | -0.243013 |
| O | 2.226010 | 1.301087 | 0.249594 |
| O | 2.226026 | -1.301082 | 0.249589 |
| C | -0.060446 | -0.000001 | -0.066778 |
| C | -0.741816 | -1.221469 | -0.042822 |
| C | -0.741819 | 1.221467 | -0.042832 |
| C | -2.124718 | -1.194546 | 0.024792 |
| H | -0.204930 | -2.170250 | -0.056056 |
| C | -2.124718 | 1.194544 | 0.024797 |
| H | -0.204923 | 2.170243 | -0.056086 |
| H | -2.746115 | -2.088374 | 0.063960 |
| H | -2.746118 | 2.088369 | 0.063980 |
| H | -3.787808 | -0.000001 | 0.107907 |
| N | -2.766053 | -0.000002 | 0.055441 |

L2-

E = -780.562031224

| Atomic symbol | x | y | z |
|---------------|-----------|-----------|-----------|
| S | 1.782850 | -0.000002 | -0.353386 |
| O | 2.171330 | 1.276145 | 0.370197 |
| O | 2.171331 | -1.276142 | 0.370210 |
| C | -0.085405 | -0.000002 | -0.110671 |
| C | -0.785546 | -1.208655 | -0.060718 |
| C | -0.785544 | 1.208654 | -0.060714 |
| C | -2.181585 | -1.211745 | 0.036296 |
| H | -0.205483 | -2.136673 | -0.062394 |
| C | -2.181582 | 1.211747 | 0.036301 |
| H | -0.205477 | 2.136669 | -0.062388 |
| H | -2.728459 | -2.158959 | 0.090879 |
| H | -2.728455 | 2.158961 | 0.090890 |
| H | -3.975269 | 0.000004 | 0.155251 |
| C | -2.884295 | 0.000001 | 0.079287 |

L2

E = -780.476096189

| Atomic symbol | x | y | z |
|---------------|-----------|-----------|-----------|
| S | 1.705674 | 0.000000 | -0.249353 |
| O | 2.207080 | 1.291879 | 0.260931 |
| O | 2.207085 | -1.291877 | 0.260923 |
| C | -0.094302 | -0.000003 | -0.080111 |
| C | -0.767652 | -1.224190 | -0.053707 |
| C | -0.767650 | 1.224189 | -0.053712 |

| | | | |
|---|-----------|-----------|-----------|
| C | -2.161149 | -1.214360 | 0.031904 |
| H | -0.203574 | -2.156644 | -0.076326 |
| C | -2.161145 | 1.214362 | 0.031899 |
| H | -0.203566 | 2.156638 | -0.076338 |
| H | -2.705666 | -2.159120 | 0.070673 |
| H | -2.705662 | 2.159121 | 0.070671 |
| H | -3.944388 | 0.000003 | 0.135383 |
| C | -2.854978 | 0.000001 | 0.072187 |

L3

E = -304.928260071

| Atomic symbol | x | y | z |
|---------------|-----------|-----------|-----------|
| C | -0.681490 | -1.218140 | -0.000000 |
| C | 0.681490 | -1.218140 | -0.000000 |
| H | -1.387591 | -2.042003 | 0.000000 |
| H | 1.387591 | -2.042003 | 0.000000 |
| C | -0.000000 | 0.987584 | 0.000001 |
| N | 1.064750 | 0.120222 | 0.000001 |
| N | -1.064750 | 0.120222 | 0.000000 |
| C | -2.445918 | 0.574146 | -0.000000 |
| H | -2.975016 | 0.216168 | 0.895947 |
| H | -2.428688 | 1.669319 | -0.000001 |
| H | -2.975014 | 0.216168 | -0.895949 |
| C | 2.445918 | 0.574146 | -0.000001 |
| H | 2.428688 | 1.669319 | 0.000004 |
| H | 2.975017 | 0.216164 | 0.895944 |
| H | 2.975012 | 0.216172 | -0.895952 |

L3+

E= -304.644468108

| Atomic symbol | x | y | z |
|---------------|-----------|-----------|-----------|
| C | -0.683360 | -1.211720 | 0.000000 |
| C | 0.683360 | -1.211720 | -0.000002 |
| H | -1.397144 | -2.028802 | 0.000012 |
| H | 1.397144 | -2.028802 | 0.000009 |
| C | 0.000000 | 0.863956 | 0.000015 |
| N | 1.102985 | 0.123022 | -0.000003 |
| N | -1.102985 | 0.123022 | -0.000001 |
| C | -2.491784 | 0.609154 | -0.000004 |
| H | -3.000913 | 0.243793 | 0.899740 |
| H | -2.477560 | 1.703588 | 0.000001 |
| H | -3.000906 | 0.243798 | -0.899755 |
| C | 2.491784 | 0.609154 | -0.000003 |
| H | 2.477561 | 1.703588 | -0.000029 |
| H | 3.000903 | 0.243817 | 0.899757 |
| H | 3.000916 | 0.243774 | -0.899738 |

L4-

E = -265.010089648

| Atomic symbol | x | y | z |
|---------------|-----------|-----------|-----------|
| C | 1.495370 | 0.578618 | -0.000009 |
| C | 0.215515 | 1.095871 | 0.000009 |
| H | 2.431986 | 1.145013 | -0.000006 |
| H | -0.165399 | 2.116692 | -0.000006 |
| C | 0.160494 | -1.218352 | 0.000006 |
| N | -0.602772 | -0.028547 | 0.000016 |
| N | 1.464437 | -0.805096 | -0.000005 |
| C | -2.041549 | -0.012670 | -0.000009 |
| H | -2.359293 | -1.067090 | 0.000022 |

| | | | |
|---|-----------|----------|-----------|
| H | -2.458981 | 0.490080 | 0.894858 |
| H | -2.458953 | 0.490008 | -0.894928 |

L4

E= -264.950527851

| Atomic symbol | x | y | z |
|---------------|-----------|-----------|-----------|
| C | 1.508481 | 0.570154 | -0.000002 |
| C | 0.227267 | 1.075003 | 0.000004 |
| H | 2.453632 | 1.104359 | -0.000010 |
| H | -0.161243 | 2.088938 | -0.000000 |
| C | 0.207771 | -1.118107 | 0.000004 |
| N | -0.621203 | -0.036990 | 0.000008 |
| N | 1.455265 | -0.826459 | -0.000003 |
| C | -2.074558 | -0.031828 | -0.000004 |
| H | -2.423439 | -1.070554 | -0.000024 |
| H | -2.460586 | 0.475018 | 0.896110 |
| H | -2.460563 | 0.475043 | -0.896114 |

L5

E = -860.897869014

| Atomic symbol | x | y | z |
|---------------|-----------|-----------|-----------|
| P | 0.068349 | 1.431410 | -0.620820 |
| C | -1.408185 | 0.380232 | -0.276720 |
| C | -1.687767 | -0.688174 | -1.148313 |
| C | -2.301397 | 0.645451 | 0.769580 |
| C | -2.816422 | -1.485159 | -0.958817 |
| H | -1.006784 | -0.901310 | -1.976967 |
| C | -3.438907 | -0.147395 | 0.956389 |
| H | -2.107353 | 1.482646 | 1.444611 |
| C | -3.697163 | -1.217030 | 0.096374 |
| H | -3.014603 | -2.316599 | -1.638311 |
| H | -4.123849 | 0.071292 | 1.778393 |
| H | -4.583626 | -1.836999 | 0.241629 |
| C | 1.411924 | 0.244004 | -0.185034 |
| C | 2.709354 | 0.561126 | -0.623128 |
| C | 1.216584 | -0.928132 | 0.561924 |
| C | 3.788942 | -0.266392 | -0.310659 |
| H | 2.867336 | 1.467439 | -1.213026 |
| C | 2.296726 | -1.760322 | 0.869969 |
| H | 0.213765 | -1.194357 | 0.900233 |
| C | 3.583924 | -1.431451 | 0.436191 |
| H | 4.791367 | -0.007285 | -0.657211 |
| H | 2.131283 | -2.668922 | 1.452729 |
| H | 4.425895 | -2.084175 | 0.674602 |
| N | 0.219182 | 2.503422 | 0.704521 |
| H | -0.231629 | 3.407597 | 0.591005 |
| H | 0.133007 | 2.145009 | 1.656415 |

L5+

E = -860.642940043

| Atomic symbol | x | y | z |
|---------------|-----------|-----------|-----------|
| P | -0.050558 | 1.150970 | -0.539754 |
| C | -1.489665 | 0.179341 | -0.147425 |
| C | -1.357726 | -1.136063 | 0.343630 |
| C | -2.767060 | 0.729425 | -0.395808 |
| C | -2.504875 | -1.876273 | 0.618649 |
| H | -0.369622 | -1.557777 | 0.529389 |
| C | -3.902229 | -0.021589 | -0.106929 |
| H | -2.868460 | 1.729563 | -0.822849 |

| | | | |
|---|-----------|-----------|-----------|
| C | -3.771855 | -1.322591 | 0.396778 |
| H | -2.411565 | -2.887390 | 1.016637 |
| H | -4.891493 | 0.399661 | -0.288557 |
| H | -4.664882 | -1.911292 | 0.611085 |
| C | 1.488833 | 0.308910 | -0.223757 |
| C | 1.861979 | -0.727374 | -1.106216 |
| C | 2.322864 | 0.680035 | 0.850002 |
| C | 3.049649 | -1.417836 | -0.881688 |
| H | 1.227646 | -0.985558 | -1.956828 |
| C | 3.512144 | -0.016026 | 1.052888 |
| H | 2.024389 | 1.481979 | 1.525641 |
| C | 3.874599 | -1.060304 | 0.192557 |
| H | 3.341449 | -2.226810 | -1.552102 |
| H | 4.156792 | 0.251016 | 1.891261 |
| H | 4.810134 | -1.596535 | 0.357725 |
| N | -0.131120 | 2.563783 | 0.338922 |
| H | -1.002705 | 2.806568 | 0.808439 |
| H | 0.424570 | 3.367617 | 0.047922 |

L6-

E = -860.309713431

| Atomic symbol | x | y | z |
|---------------|-----------|-----------|-----------|
| P | -0.032980 | 1.349930 | -0.954553 |
| C | -1.380997 | 0.201073 | -0.305794 |
| C | -1.474926 | -1.180281 | -0.565153 |
| C | -2.436042 | 0.797484 | 0.409849 |
| C | -2.563612 | -1.933167 | -0.120062 |
| H | -0.673000 | -1.682749 | -1.111780 |
| C | -3.531122 | 0.050185 | 0.854826 |
| H | -2.369924 | 1.874782 | 0.595728 |
| C | -3.603648 | -1.322753 | 0.594915 |
| H | -2.601185 | -3.007714 | -0.325661 |
| H | -4.333714 | 0.541884 | 1.414104 |
| H | -4.457443 | -1.910939 | 0.941629 |
| C | 1.386700 | 0.301099 | -0.292177 |
| C | 1.855388 | -0.848983 | -0.954562 |
| C | 2.109238 | 0.745731 | 0.827705 |
| C | 2.966881 | -1.557103 | -0.488381 |
| H | 1.351939 | -1.181471 | -1.868053 |
| C | 3.222843 | 0.045965 | 1.299624 |
| H | 1.784104 | 1.676093 | 1.305750 |
| C | 3.655316 | -1.116996 | 0.649232 |
| H | 3.307187 | -2.451540 | -1.019707 |
| H | 3.761245 | 0.407393 | 2.181769 |
| H | 4.530657 | -1.662438 | 1.011639 |
| N | -0.116603 | 2.771037 | -0.161204 |
| H | -0.225056 | 2.656963 | 0.861161 |

L6

E = -860.248419747

| Atomic symbol | x | y | z |
|---------------|-----------|-----------|-----------|
| P | 0.065280 | 1.266628 | -0.682031 |
| C | -1.451764 | 0.349330 | -0.225084 |
| C | -2.054076 | -0.525963 | -1.142664 |
| C | -2.034889 | 0.540704 | 1.038998 |
| C | -3.212975 | -1.222453 | -0.791150 |
| H | -1.616395 | -0.653527 | -2.135631 |
| C | -3.198657 | -0.149451 | 1.381497 |
| H | -1.564506 | 1.225258 | 1.747608 |

| | | | |
|---|-----------|-----------|-----------|
| C | -3.786320 | -1.033913 | 0.470054 |
| H | -3.675344 | -1.905283 | -1.506409 |
| H | -3.646542 | -0.002049 | 2.366254 |
| H | -4.695928 | -1.572525 | 0.741842 |
| C | 1.455183 | 0.202459 | -0.210994 |
| C | 1.355442 | -1.197299 | -0.276287 |
| C | 2.675359 | 0.797726 | 0.154028 |
| C | 2.460509 | -1.991807 | 0.032545 |
| H | 0.407602 | -1.665860 | -0.547824 |
| C | 3.774230 | -0.004596 | 0.463375 |
| H | 2.738438 | 1.885438 | 0.209709 |
| C | 3.672339 | -1.398698 | 0.401202 |
| H | 2.372961 | -3.079155 | -0.009168 |
| H | 4.716383 | 0.461713 | 0.758212 |
| H | 4.535301 | -2.022035 | 0.642167 |
| N | 0.292922 | 2.690131 | 0.033790 |
| H | -0.527897 | 3.301438 | -0.045951 |

L7-

E = -409.330349942

| Atomic symbol | x | y | z |
|---------------|-----------|-----------|-----------|
| Si | -0.000003 | 0.000000 | -0.703103 |
| C | 0.765438 | -1.513206 | 0.297704 |
| H | 1.832663 | -1.657229 | 0.048659 |
| H | 0.693207 | -1.370327 | 1.397546 |
| H | 0.249057 | -2.458240 | 0.048711 |
| C | 0.927762 | 1.419488 | 0.297704 |
| H | 2.004372 | 1.444813 | 0.048696 |
| H | 0.518871 | 2.415745 | 0.048673 |
| H | 0.840162 | 1.285479 | 1.397548 |
| C | -1.693197 | 0.093718 | 0.297708 |
| H | -2.351541 | -0.758509 | 0.048652 |
| H | -1.533345 | 0.084824 | 1.397551 |
| H | -2.253425 | 1.013438 | 0.048717 |

L7

E = -409.302934261

| Atomic symbol | x | y | z |
|---------------|-----------|-----------|-----------|
| Si | 0.000001 | 0.000002 | -0.426861 |
| C | 1.577810 | 0.852383 | 0.177314 |
| H | 1.631153 | 1.892389 | -0.176444 |
| H | 1.607907 | 0.868599 | 1.281088 |
| H | 2.476882 | 0.326946 | -0.176503 |
| C | -1.527092 | 0.940231 | 0.177313 |
| H | -1.521609 | 1.981558 | -0.176537 |
| H | -2.454436 | 0.466399 | -0.176407 |
| H | -1.556159 | 0.958222 | 1.281088 |
| C | -0.050719 | -1.792616 | 0.177312 |
| H | 0.823296 | -2.358806 | -0.176421 |
| H | -0.051754 | -1.826795 | 1.281087 |
| H | -0.955282 | -2.308525 | -0.176531 |

L8-

E = -92.8905318756

| Atomic symbol | x | y | z |
|---------------|-----------|-----------|-----------|
| C | -0.000000 | -0.000000 | -0.636718 |
| N | 0.000000 | 0.000000 | 0.545759 |

L8

E = -92.7525610350

| Atomic symbol | x | y | z |
|---------------|-----------|-----------|-----------|
| C | 0.000000 | 0.000000 | -0.632815 |
| N | -0.000000 | -0.000000 | 0.542413 |

L9

E = -1036.65693680

| Atomic symbol | x | y | z |
|---------------|-----------|-----------|-----------|
| P | 0.000762 | 0.000048 | -1.280953 |
| C | -1.070775 | 1.246092 | -0.450271 |
| C | -1.872242 | 0.972964 | 0.668874 |
| C | -1.071975 | 2.546312 | -0.986038 |
| C | -2.652056 | 1.981027 | 1.243453 |
| H | -1.883432 | -0.031950 | 1.093244 |
| C | -1.838730 | 3.555706 | -0.402203 |
| H | -0.462018 | 2.764622 | -1.866521 |
| C | -2.633825 | 3.274227 | 0.714254 |
| H | -3.272519 | 1.754535 | 2.113064 |
| H | -1.823889 | 4.562425 | -0.824516 |
| H | -3.241674 | 4.060350 | 1.165934 |
| C | -0.543901 | -1.550499 | -0.450729 |
| C | -1.670783 | -2.199512 | -0.985480 |
| C | 0.094902 | -2.109715 | 0.666328 |
| C | -2.163060 | -3.367572 | -0.401035 |
| H | -2.164930 | -1.778899 | -1.865153 |
| C | -0.389334 | -3.288532 | 1.241115 |
| H | 0.972842 | -1.618689 | 1.088705 |
| C | -1.520848 | -3.916966 | 0.713948 |
| H | -3.043716 | -3.856497 | -0.822342 |
| H | 0.117629 | -3.714049 | 2.109649 |
| H | -1.898704 | -4.835865 | 1.166027 |
| C | 1.615655 | 0.304303 | -0.450486 |
| C | 1.778996 | 1.133189 | 0.670373 |
| C | 2.742347 | -0.343245 | -0.987269 |
| C | 3.041526 | 1.303748 | 1.245427 |
| H | 0.913969 | 1.645415 | 1.094371 |
| C | 3.999713 | -0.184561 | -0.402908 |
| H | 2.626668 | -0.978631 | -1.869221 |
| C | 4.152897 | 0.642636 | 0.714986 |
| H | 3.155432 | 1.952746 | 2.116214 |
| H | 4.864454 | -0.699079 | -0.826645 |
| H | 5.137414 | 0.775220 | 1.167447 |

L9+

E = -1036.40388816

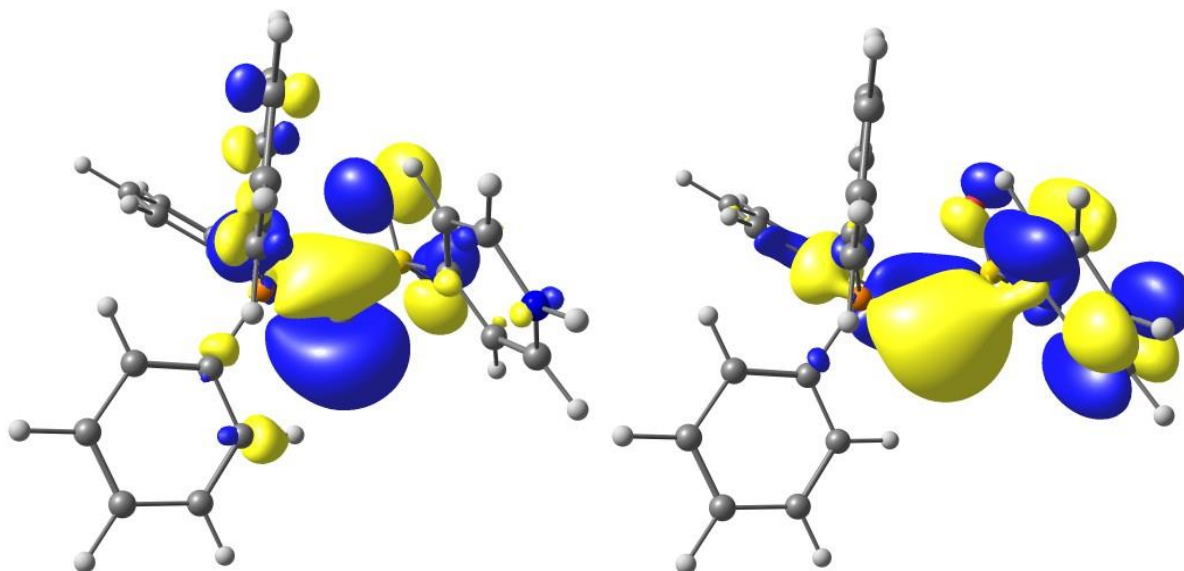
| Atomic symbol | x | y | z |
|---------------|-----------|-----------|-----------|
| P | 0.000060 | 0.000021 | -0.714586 |
| C | -0.750738 | 1.545580 | -0.252741 |
| C | -1.898152 | 1.589722 | 0.567528 |
| C | -0.189266 | 2.739811 | -0.759686 |
| C | -2.455311 | 2.822815 | 0.895640 |
| H | -2.328235 | 0.668207 | 0.960399 |
| C | -0.756156 | 3.963483 | -0.418240 |
| H | 0.679471 | 2.702102 | -1.419641 |
| C | -1.888611 | 4.006319 | 0.405839 |
| H | -3.331511 | 2.863301 | 1.543910 |
| H | -0.323987 | 4.887198 | -0.804492 |
| H | -2.334355 | 4.967828 | 0.664338 |
| C | -0.963110 | -1.422893 | -0.252777 |

| | | | |
|---|-----------|-----------|-----------|
| C | -2.277944 | -1.533824 | -0.760048 |
| C | -0.427861 | -2.438574 | 0.567722 |
| C | -3.054357 | -2.636551 | -0.418634 |
| H | -2.679382 | -0.762731 | -1.420285 |
| C | -1.217330 | -3.537535 | 0.895905 |
| H | 0.585123 | -2.350313 | 0.960891 |
| C | -2.525480 | -3.638549 | 0.405784 |
| H | -4.070300 | -2.724207 | -0.805139 |
| H | -0.814466 | -4.316448 | 1.544453 |
| H | -3.135435 | -4.505245 | 0.664245 |
| C | 1.713876 | -0.122691 | -0.252593 |
| C | 2.326069 | 0.849078 | 0.567350 |
| C | 2.467211 | -1.206272 | -0.759341 |
| C | 3.672576 | 0.714965 | 0.895236 |
| H | 1.743183 | 1.682407 | 0.960163 |
| C | 3.810450 | -1.327217 | -0.418130 |
| H | 1.999977 | -1.940022 | -1.418863 |
| C | 4.414016 | -0.367689 | 0.405520 |
| H | 4.145868 | 1.453568 | 1.543382 |
| H | 4.394191 | -2.163487 | -0.804265 |
| H | 5.469656 | -0.462344 | 0.663705 |

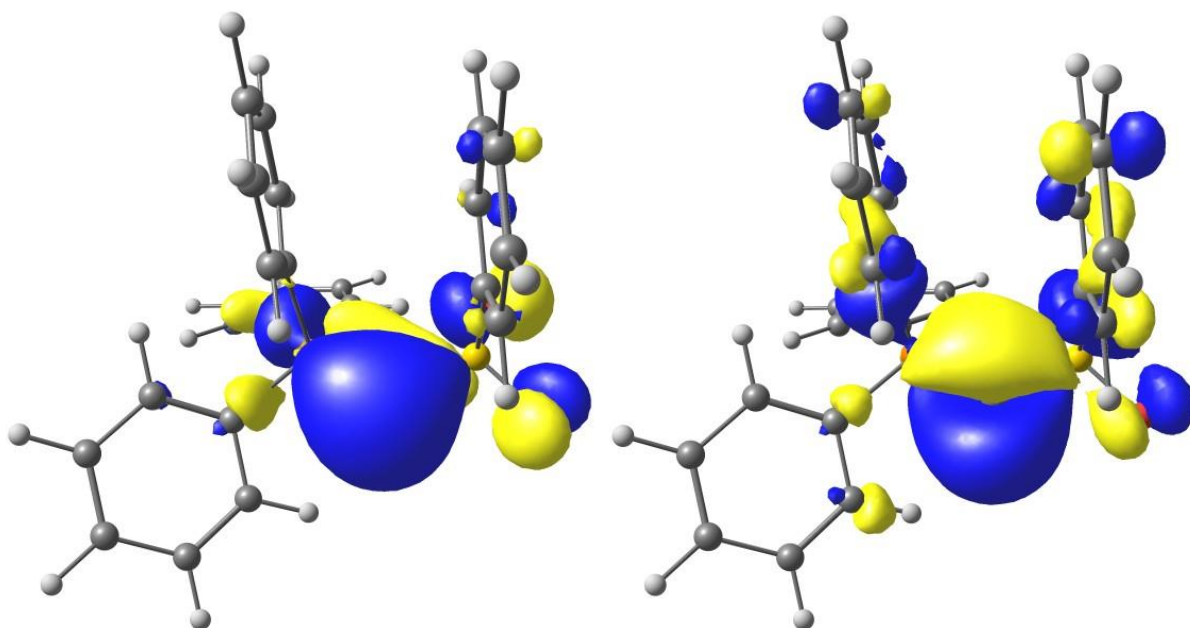
2. Canonical Orbitals

HOMO (left), HOMO-1 (right) for 1-9. Orbitals are taken from BP86-D3(BJ)/Def2TZVP calculations.

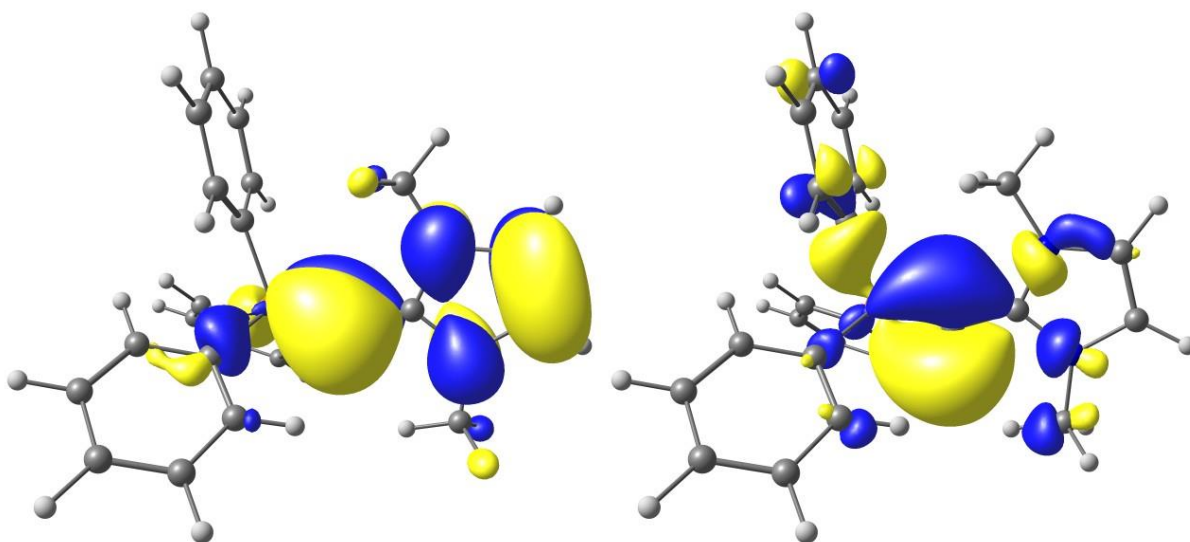
1:



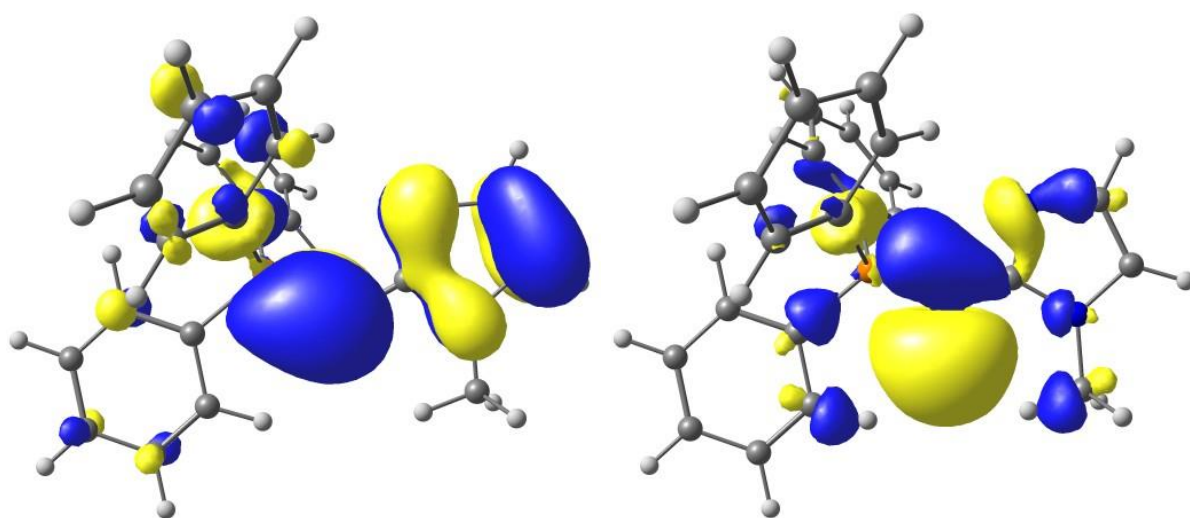
2:



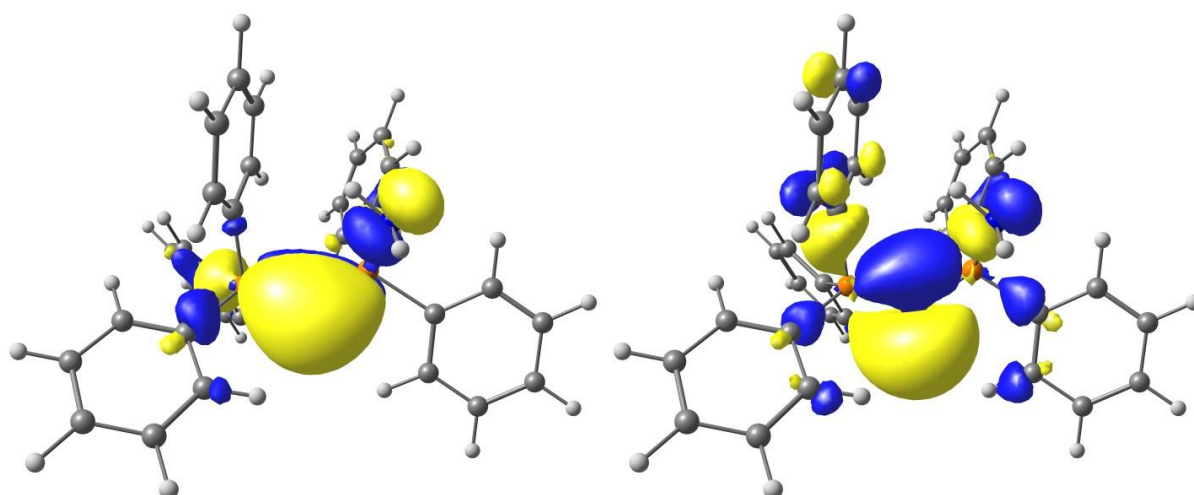
3:



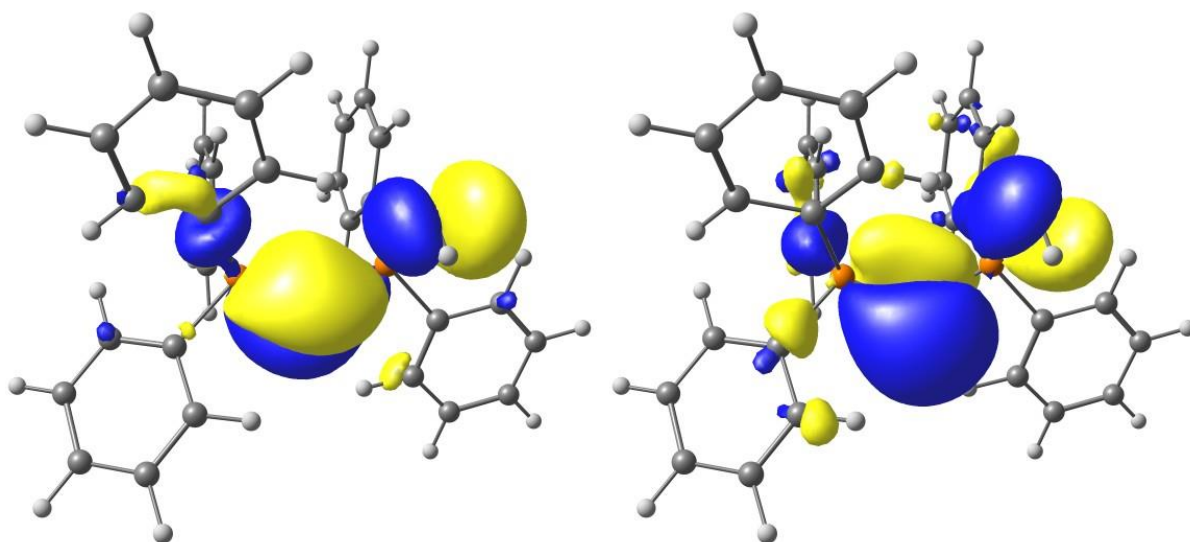
4:



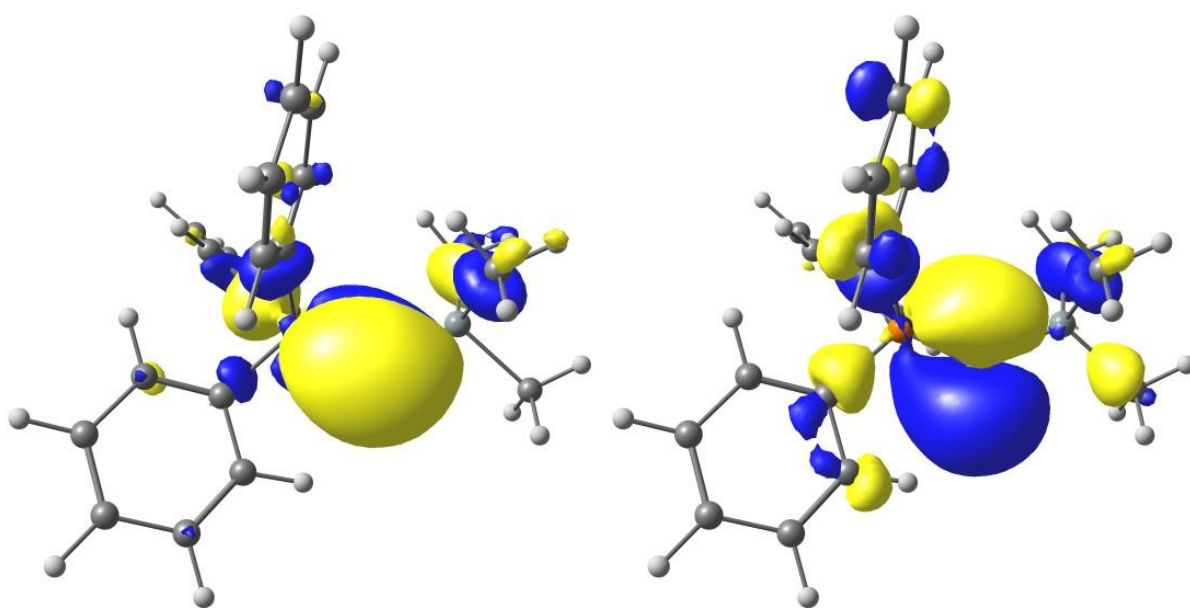
5:



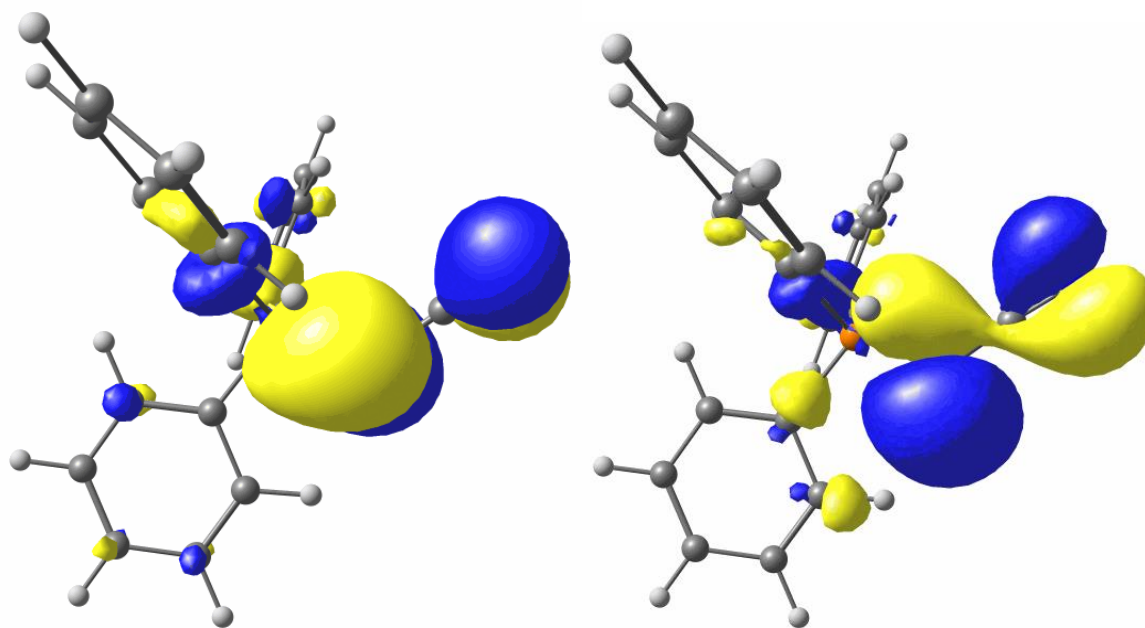
6:



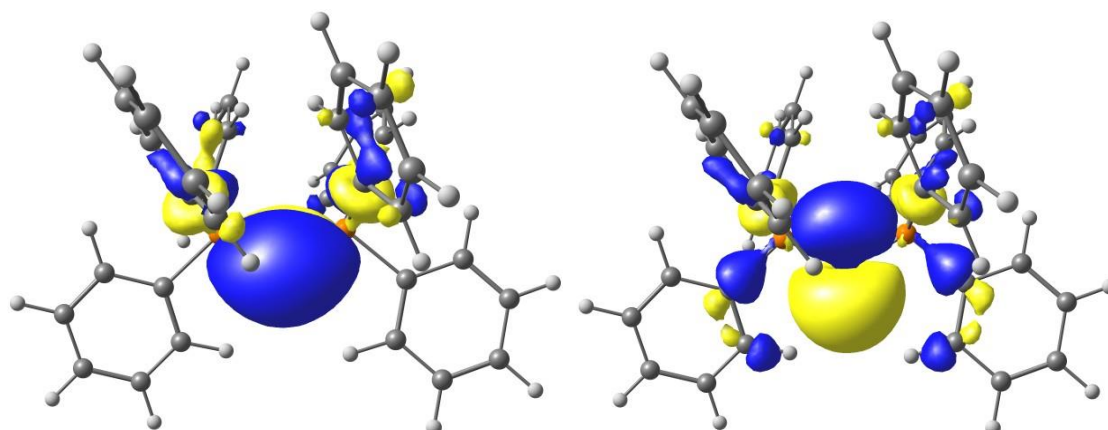
7:



8:



9:



3. EDA tables

All energies are given in kcal/mol and taken from BP86/TZ2P ADF calculations.

| 3 | dada | dodo | ylyl | yldo | doyl | dayl | ylda | dado | doda |
|--|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| ΔE_{Int} | -199.5 | -482.0 | -669.0 | -388.7 | -441.9 | -352.7 | -336.8 | -250.2 | -287.5 |
| ΔE_{Pauli} | 951.5 | 476.4 | 1044.8 | 945.0 | 917.5 | 785.4 | 932.6 | 747.5 | 873.0 |
| ΔE_{elstat} | -401.5 | -380.4 | -953.1 | -642.3 | -655.0 | -457.5 | -516.8 | -307.7 | -382.0 |
| ΔE_{Orb} | -749.5 | -578.0 | -760.7 | -691.4 | -704.4 | -680.6 | -752.6 | -690.0 | -778.5 |
| $\Delta E_{\text{prep}}(\text{PPh}_3)$ | 0.9 | 128.1 | 14.4 | 14.4 | 128.1 | 0.9 | 14.4 | 0.9 | 128.1 |
| $\Delta E_{\text{prep}}(\text{L})$ | 2.7 | 91.4 | 10.1 | 91.4 | 10.1 | 10.1 | 2.7 | 91.4 | 2.7 |
| $\Delta E_{\text{prep}}(\text{C})$ | 43.5 | 100.8 | 0.0 | 0.0 | 0.0 | 41.0 | 41.0 | 0.0 | 0.0 |
| ΔE_{prep} | 47.1 | 320.3 | 24.4 | 105.8 | 138.1 | 52.0 | 58.0 | 92.3 | 130.8 |

| BDE | 152.5 | 152.5 | 640.2 | 277.1 | 297.2 | 297.2 | 277.1 | 152.5 | 152.5 |
|--|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| 4 | dada | dodo | ylyl | yldo | doyl | dayl | ylda | dado | doda |
| ΔE_{Int} | -219.4 | -487.1 | -548.7 | -396.4 | -319.0 | -232.6 | -356.7 | -258.1 | -304.7 |
| ΔE_{Pauli} | 866.7 | 517.6 | 1018.4 | 928.9 | 914.8 | 797.3 | 931.5 | 761.3 | 874.9 |
| ΔE_{elstat} | -399.4 | -400.0 | -797.9 | -605.3 | -555.4 | -411.3 | -535.5 | -367.3 | -448.0 |
| ΔE_{Orb} | -686.8 | -604.6 | -769.2 | -720.0 | -678.3 | -618.5 | -752.7 | -652.0 | -731.7 |
| $\Delta E_{\text{prep}}(\text{PPh}_3)$ | 0.7 | 127.4 | 14.2 | 14.2 | 127.4 | 0.7 | 14.2 | 0.7 | 127.4 |
| $\Delta E_{\text{prep}}(\text{L})$ | 0.9 | 75.3 | 7.6 | 75.3 | 7.6 | 7.6 | 0.9 | 75.3 | 0.9 |
| $\Delta E_{\text{prep}}(\text{C})$ | 43.5 | 100.8 | 0.0 | 0.0 | 0.0 | 41.0 | 41.0 | 0.0 | 0.0 |
| ΔE_{prep} | 45.2 | 303.5 | 21.8 | 89.5 | 135.0 | 49.3 | 56.1 | 76.0 | 128.3 |
| BDE | 174.4 | 174.4 | 522.4 | 299.0 | 179.4 | 179.4 | 299.0 | 174.4 | 174.4 |
| 5 | dada | dodo | ylyl | yldo | doyl | dayl | ylda | dado | doda |
| ΔE_{Int} | -181.4 | -470.1 | -628.1 | -376.2 | -401.6 | -314.4 | -316.3 | -240.3 | -267.6 |
| ΔE_{Pauli} | 786.3 | 580.0 | 1048.6 | 968.3 | 934.5 | 818.5 | 841.5 | 798.1 | 788.2 |
| ΔE_{elstat} | -357.0 | -414.1 | -988.5 | -695.8 | -683.1 | -548.9 | -550.2 | -390.4 | -385.6 |
| ΔE_{Orb} | -610.7 | -636.1 | -688.2 | -648.7 | -652.9 | -584.0 | -607.6 | -647.9 | -670.3 |
| $\Delta E_{\text{prep}}(\text{PPh}_3)$ | 1.0 | 124.9 | 11.9 | 11.9 | 124.9 | 1.0 | 11.9 | 1.0 | 124.9 |
| $\Delta E_{\text{prep}}(\text{L})$ | 4.2 | 103.8 | 10.2 | 103.8 | 10.2 | 10.2 | 4.2 | 103.8 | 4.2 |
| $\Delta E_{\text{prep}}(\text{C})$ | 43.5 | 100.8 | 0.0 | 0.0 | 0.0 | 41.0 | 41.0 | 0.0 | 0.0 |
| ΔE_{prep} | 48.7 | 329.5 | 22.1 | 115.7 | 135.1 | 52.2 | 57.1 | 104.7 | 129.0 |
| BDE | 133.0 | 133.0 | 603.4 | 257.6 | 260.4 | 260.4 | 257.6 | 133.0 | 133.0 |
| 6 | dada | dodo | ylyl | yldo | doyl | dayl | ylda | dado | doda |
| ΔE_{Int} | -190.5 | -478.2 | -513.7 | -388.4 | -283.0 | -197.0 | -328.2 | -249.6 | -275.4 |
| ΔE_{Pauli} | 776.6 | 662.1 | 1052.2 | 1036.8 | 950.5 | 798.7 | 822.9 | 849.5 | 900.2 |
| ΔE_{elstat} | -351.7 | -481.7 | -861.9 | -713.6 | -597.5 | -437.6 | -507.7 | -432.4 | -463.2 |
| ΔE_{Orb} | -615.5 | -658.5 | -703.9 | -711.6 | -636.1 | -558.2 | -643.4 | -666.6 | -712.4 |
| $\Delta E_{\text{prep}}(\text{PPh}_3)$ | 0.3 | 123.6 | 14.3 | 14.3 | 123.6 | 0.3 | 14.3 | 0.3 | 123.6 |
| $\Delta E_{\text{prep}}(\text{L})$ | 3.2 | 99.2 | 3.8 | 99.2 | 3.8 | 3.8 | 3.2 | 99.2 | 3.2 |
| $\Delta E_{\text{prep}}(\text{C})$ | 43.5 | 100.8 | 0.0 | 0.0 | 0.0 | 41.0 | 41.0 | 0.0 | 0.0 |
| ΔE_{prep} | 47.1 | 323.6 | 18.1 | 113.5 | 127.4 | 45.2 | 58.5 | 99.5 | 126.8 |
| BDE | 143.5 | 143.5 | 492.8 | 268.1 | 149.7 | 149.7 | 268.1 | 143.5 | 143.5 |

| 7 | dada | dodo | yllyl | ylldo | doysl | dayl | yllda | dado | doda |
|--|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| ΔE_{Int} | -218.0 | -466.0 | -522.1 | -375.9 | -291.9 | -202.7 | -358.6 | -234.2 | -306.1 |
| ΔE_{Pauli} | 775.5 | 465.5 | 901.0 | 849.2 | 791.0 | 680.2 | 815.0 | 682.1 | 773.2 |
| ΔE_{elstat} | -369.2 | -375.0 | -792.8 | -598.6 | -530.0 | -388.0 | -499.0 | -334.5 | -399.2 |
| ΔE_{Orb} | -624.3 | -556.6 | -630.3 | -626.5 | -552.8 | -494.9 | -674.6 | -581.9 | -680.1 |
| $\Delta E_{\text{prep}}(\text{PPh}_3)$ | 1.3 | 128.4 | 18.1 | 18.1 | 128.4 | 1.3 | 18.1 | 1.3 | 128.4 |
| $\Delta E_{\text{prep}}(\text{L})$ | 4.2 | 60.9 | 3.0 | 60.9 | 3.0 | 3.0 | 4.2 | 60.9 | 4.2 |
| $\Delta E_{\text{prep}}(\text{C})$ | 43.5 | 100.8 | 0.0 | 0.0 | 0.0 | 41.0 | 41.0 | 0.0 | 0.0 |
| ΔE_{prep} | 49.0 | 290.2 | 21.1 | 79.0 | 131.5 | 45.3 | 63.3 | 62.2 | 132.6 |
| BDE | 169.1 | 169.1 | 498.3 | 293.7 | 155.3 | 155.3 | 293.7 | 169.1 | 169.1 |

| 8 | dada | dodo | yllyl | ylldo | doysl | dayl | yllda | dado | doda |
|--|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| ΔE_{Int} | -205.7 | -526.3 | -572.4 | -435.2 | -343.1 | -256.0 | -343.2 | -296.6 | -291.7 |
| ΔE_{Pauli} | 842.4 | 509.4 | 950.8 | 918.2 | 864.3 | 753.6 | 886.6 | 766.4 | 834.1 |
| ΔE_{elstat} | -374.4 | -396.4 | -769.9 | -573.1 | -527.2 | -387.4 | -485.1 | -363.3 | -404.2 |
| ΔE_{Orb} | -673.7 | -639.2 | -753.3 | -780.4 | -680.1 | -622.2 | -744.7 | -699.7 | -721.6 |
| $\Delta E_{\text{prep}}(\text{PPh}_3)$ | 0.6 | 127.5 | 14.4 | 14.4 | 127.5 | 0.6 | 14.4 | 0.6 | 127.5 |
| $\Delta E_{\text{prep}}(\text{L})$ | 0.1 | 131.0 | 0.4 | 131.0 | 0.4 | 0.4 | 0.1 | 131.0 | 0.1 |
| $\Delta E_{\text{prep}}(\text{C})$ | 43.5 | 100.8 | 0.0 | 0.0 | 0.0 | 41.0 | 41.0 | 0.0 | 0.0 |
| ΔE_{prep} | 44.3 | 359.2 | 14.8 | 145.3 | 127.9 | 42.1 | 55.5 | 131.6 | 127.6 |
| BDE | 161.5 | 161.5 | 554.4 | 286.1 | 211.4 | 211.4 | 286.1 | 161.5 | 161.5 |

| 9 | dada | dodo | yllyl | ylldo | doysl | dayl | yllda | dado | doda |
|--|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| ΔE_{Int} | -170.6 | -486.3 | -618.0 | -392.0 | -392.0 | -304.9 | -304.9 | -256.6 | -256.6 |
| ΔE_{Pauli} | 770.4 | 571.1 | 1054.4 | 950.6 | 950.6 | 820.1 | 820.1 | 779.1 | 779.1 |
| ΔE_{elstat} | -341.4 | -403.6 | -970.7 | -678.1 | -678.1 | -532.8 | -532.8 | -373.2 | -373.2 |
| ΔE_{Orb} | -599.6 | -653.8 | -701.8 | -664.5 | -664.5 | -592.2 | -592.2 | -662.6 | -662.6 |
| $\Delta E_{\text{prep}}(\text{PPh}_3)$ | 1.1 | 126.7 | 11.5 | 11.5 | 126.7 | 1.1 | 11.5 | 1.1 | 126.7 |
| $\Delta E_{\text{prep}}(\text{L})$ | 1.1 | 126.7 | 11.5 | 126.7 | 11.5 | 11.5 | 1.1 | 126.7 | 1.1 |
| $\Delta E_{\text{prep}}(\text{C})$ | 43.5 | 100.8 | 0.0 | 0.0 | 0.0 | 41.0 | 41.0 | 0.0 | 0.0 |
| ΔE_{prep} | 45.7 | 354.2 | 23.0 | 138.2 | 138.2 | 53.6 | 53.6 | 127.8 | 127.8 |
| BDE | 124.9 | 124.9 | 592.5 | 249.5 | 249.5 | 249.5 | 249.5 | 124.9 | 124.9 |

4. Nalewajski-Mrozek bond orders and NBO analysis data

Nalewajski-Mrozek bond orders

| | L | NMBI | |
|---|----------------------------------|------|------|
| | | C-P | C-E |
| 1 | SO ₂ PyH | 1.30 | 1.03 |
| 2 | SO ₂ Ph ⁻ | 1.57 | 1.12 |
| 3 | IMe | 1.46 | 1.80 |
| 4 | IMe ⁻ | 1.48 | 1.56 |
| 5 | PPh ₂ NH ₂ | 1.48 | 1.48 |
| 6 | PPh ₂ NH ⁻ | 1.62 | 1.24 |
| 7 | SiMe ₃ ⁻ | 1.72 | 1.25 |
| 8 | CN ⁻ | 1.39 | 1.67 |
| 9 | PPh ₃ | 1.47 | 1.47 |

NBO analysis data

| | L | Occ | C-P(σ) | | C-P(π) | | C-E(σ) | | | C-E(π) | |
|---|----------------------------------|------|-----------------|------|--------------|------|-----------------|------|------|--------------|------|
| | | | %(C) | %(s) | Occ | %(C) | Occ | %(C) | %(s) | Occ | %(C) |
| 1 | SO ₂ PyH | 1.96 | 55.4 | 28.6 | | | 1.96 | 50.5 | 24.3 | | |
| 2 | SO ₂ Ph ⁻ | 1.96 | 55.8 | 30.7 | 1.63 | 87.6 | 1.97 | 50.6 | 26.0 | | |
| 3 | IMe | 1.96 | 58.1 | 37.3 | | | 1.98 | 46.8 | 45.8 | 1.84 | 61.9 |
| 4 | IMe ⁻ | 1.95 | 55.2 | 28.5 | | | 1.97 | 46.4 | 35.5 | | |
| 5 | PPh ₂ NH ₂ | 1.96 | 57.2 | 30.9 | | | 1.96 | 58.2 | 31.8 | 1.65 | 88.9 |
| 6 | PPh ₂ NH ⁻ | 1.96 | 56.7 | 32.1 | 1.64 | 87.2 | 1.95 | 59.4 | 31.2 | | |
| 7 | SiMe ₃ ⁻ | 1.96 | 55.8 | 31.0 | 1.66 | 84.4 | 1.92 | 70.4 | 27.6 | | |
| 8 | CN ⁻ | 1.92 | 59.7 | 49.7 | 1.64 | 88.7 | 1.99 | 49.0 | 41.8 | | |
| 9 | PPh ₃ | 1.96 | 57.5 | 30.5 | 1.62 | 90.4 | 1.96 | 57.4 | 30.4 | | |